# LDRD Day


Laboratory Directed Research and Development

Los Alamos National Laboratory

September 8, 2010

**Energy Security** **Nuclear Security**

**Global Security** **Scientific Discovery**

**Innovation for Our Nation**

LDRD innovation for our nation

Los Alamos NATIONAL LABORATORY EST. 1943

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LA-UR 10-05560

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## Global Security



## Scientific Discovery

LDRD

## Message from the LDRD Program Director

America faces energy, security, economic, and environmental challenges that, in their scope and complexity, are perhaps unparalleled in the nation's history. Los Alamos National Laboratory is called upon to respond to those challenges; as a premier national security science laboratory, our Federal sponsors (and others) count on us to address these challenges by technical means.

Congress has authorized the national laboratories to invest in technical capabilities and new mission solutions through the Laboratory Directed Research and Development (LDRD) program. LDRD supports the most advanced, high-risk ideas at Los Alamos. Many of the Laboratory's successes, which range from the heavens (the Earth's radiation belts and their effects on satellites) to the Earth (the accelerated cleanup of the Rocky Flats site near Denver), can be traced to LDRD.

LDRD investments are rigorously selected, based on the independent judgments of leading scientists and engineers, inside and outside the Laboratory. LDRD is a small fraction of the Laboratory budget, capped at 8 percent for National Nuclear Security Administration laboratories.  In a nutshell, LDRD is how the Laboratory steps into action to build the future of its science and technology.

That future revolves around the national challenges in energy security, nuclear security, and global security, and is driven forward by the engine of scientific discovery. At LDRD Day, we showcase the ideas being pursued by some of the leading scientists and engineers of the Laboratory. What you will see is a small sample of the excitement of LDRD, but enough to give a feel of the breadth and quality of the work. This select research is one of the best ways to understand the future of what Los Alamos will deliver to the nation.

**Dr. William Priedhorsky**
*LDRD Program Director*
*Los Alamos National Laboratory*

William Priedhorsky received a bachelor's degree in physics *summa cum laude* and Phi Beta Kappa from Whitman College in 1973, and a Ph.D. in physics, specializing in x-ray astronomy, from the California Institute of Technology in 1978.  Since joining Los Alamos National Laboratory as a staff member in 1978, his research has spanned the gamut from development of time-resolved, spectral, and imaging x-ray instrumentation, to new technologies to stymie the spread of weapons of mass destruction.  He has earned numerous awards for distinguished performance in his career, most recently an honorary degree of humane letters from Whitman College.

# Invited Speakers

## Charles F. McMillan

*Principal Associate Director for Weapons Programs*

*Los Alamos National Laboratory*

Leading the weapons programs organization at Los Alamos, Charles McMillan directs the science, technology, engineering, and infrastructure that enables the Laboratory's core mission of ensuring the safety, reliability, and performance of the nation's nuclear deterrent.

McMillan has more than 22 years of scientific and management experience in weapons science and stockpile certification and hands-on experience in both experimental physics and computational science. As a manager of experimental facilities, he has demonstrated experience in successfully balancing mission performance with security and safety.

PADWP consists of two associate directorates, Weapons, and Stockpile Manufacturing & Support. A wide variety of work is accomplished in these organizations ranging from applied physics to hydrodynamic experiments to plutonium science, manufacturing & technology.

"I have great optimism for the future," said McMillan. "This is a complicated time, but also a time of great opportunity for the program, an opportunity to work with the Administration to shape tomorrow's nuclear security complex while effectively managing the nuclear stockpile along the way. The service we provide to the nation is just as important now as it ever was."

The principal associate directorate includes weapons scientists and engineers who perform design, simulation, and experiments to support the technical analysis necessary to ensure stockpile remains safe, secure and reliable. This also includes small-scale materials experiments thru fully integrated hydrotests that provide essential validation data for modeling and simulation, allowing the Laboratory to rely on predictive-science and "Quantifying Margins and Uncertainties"-based capability for the stockpile, in the absence of nuclear testing.

McMillan has led the Laboratory's weapons physics organization since 2006, when Los Alamos National Security, LLC, began managing the Laboratory. Prior to joining the Laboratory, McMillan served in a variety of research and management positions at Lawrence Livermore National Laboratory.

He holds a bachelor's degree in mathematics and physics from Columbia Union College and a doctorate in physics from the Massachusetts Institute of Technology. He has been awarded two DOE Awards of Excellence, one of which was presented for development of an innovative holographic tool that enhances the ability to predict nuclear performance.

## Alan Bishop

*Associate Director for Theory, Simulation, and Computation*

*Los Alamos National Laboratory*

Alan Bishop is an internationally recognized leader in condensed matter theory, statistical physics and nonlinear physics. He has made major contributions in the areas of solitons, quantum complexity, structural and magnetic transitions, collective excitations in lowdimensional organic and inorganic materials and complex electronic materials with strong spin-charge-lattice coupling. He is a Fellow of the American Physical Society, Fellow of the American Association for the Advancement of Science, a recipient of the Department of Energy's E.O. Lawrence Award, a Humboldt Senior Fellow, and a Laboratory Fellow.

A proud naturalized U.S. citizen, Alan was born in Staffordshire, England, and was educated at the University of East Anglia and the University of Cambridge where he earned a doctorate degree in Theoretical Solid State Physics at the Cavendish Laboratory– in between much mountaineering in Scotland and gaining a "blue" for Judo at Cambridge! After periods at Oxford, Cornell, and London Universities, he came to work at Los Alamos Scientific Laboratory (LASL) in January 1979 taking a staff position in the Materials and Statistical Physics Theory Group of the Theoretical Division. After a two-year stint as the Acting/ Deputy Chairman of the Center for Nonlinear Studies and fourteen years as the Group Leader of the Condensed Matter Theory Group at Los Alamos, he became the Leader of the Theoretical Division in August 1999.

With the transition from the University of California to Los Alamos National Security, LLC, management of Los Alamos National Laboratory (LANL) on June 1 2006, Alan was selected to become the first Associate Director for Theory, Simulation, and Computation. Under his leadership, the directorate oversees an annual budget of $350M and over 1200 employees within three divisions: Computer, Computational, and Statistical Sciences (CCS); High Performance Computing (HPC), and Theoretical (T) divisions.

## Heather Wilson

*NM Congresswoman, 1998-2009*

For ten years, Congresswoman Heather Wilson helped shape key legislation that cemented our national security, improved our domestic energy policy, and reformed American healthcare. A senior member of the House Energy and Commerce Committee and the House Permanent Select Committee on Intelligence--and the only female veteran in Congress--she was also one of the top House members on the topics of Medicaid and Medicare, energy, and national security.

House Republican leaders frequently turned to her because of her ability to effectively and passionately communicate why reform matters to people.

A recipient of numerous public service awards for protecting taxpayers and promoting free enterprise, Wilson received Distinguished Public Service Awards from the CIA and the Director of National Intelligence upon leaving the Congress.

**A Life of Service**

Wilson's record of public service dates to age 17, when she packed her bags for the U.S. Air Force Academy in the third class to include women. She graduated in 1982, and eventually became the first Air Force Academy graduate to serve in Congress. A Rhodes Scholar, Wilson earned her master's and doctoral degrees in international relations from Oxford University in England.

As an Air Force officer she worked with our NATO allies and in the United Kingdom. Then in 1989, she became director for European defense policy and arms control on the National Security Council staff at the White House under the first President Bush.

**An Advocate for Families**

Wilson was the owner of a successful small business in Albuquerque when, in 1995, she was asked to take charge of New Mexico's Children, Youth and Families Department where she led efforts to reform child welfare laws, modernize the juvenile justice system and improve early childhood education.

Wilson now works as a senior advisor to several large defense and scientific institutions.

Wilson is married to Jay Hone, an Albuquerque attorney. They have one grown son and two school-age children, Joshua and Caitlin Hone.

## Herb Funsten

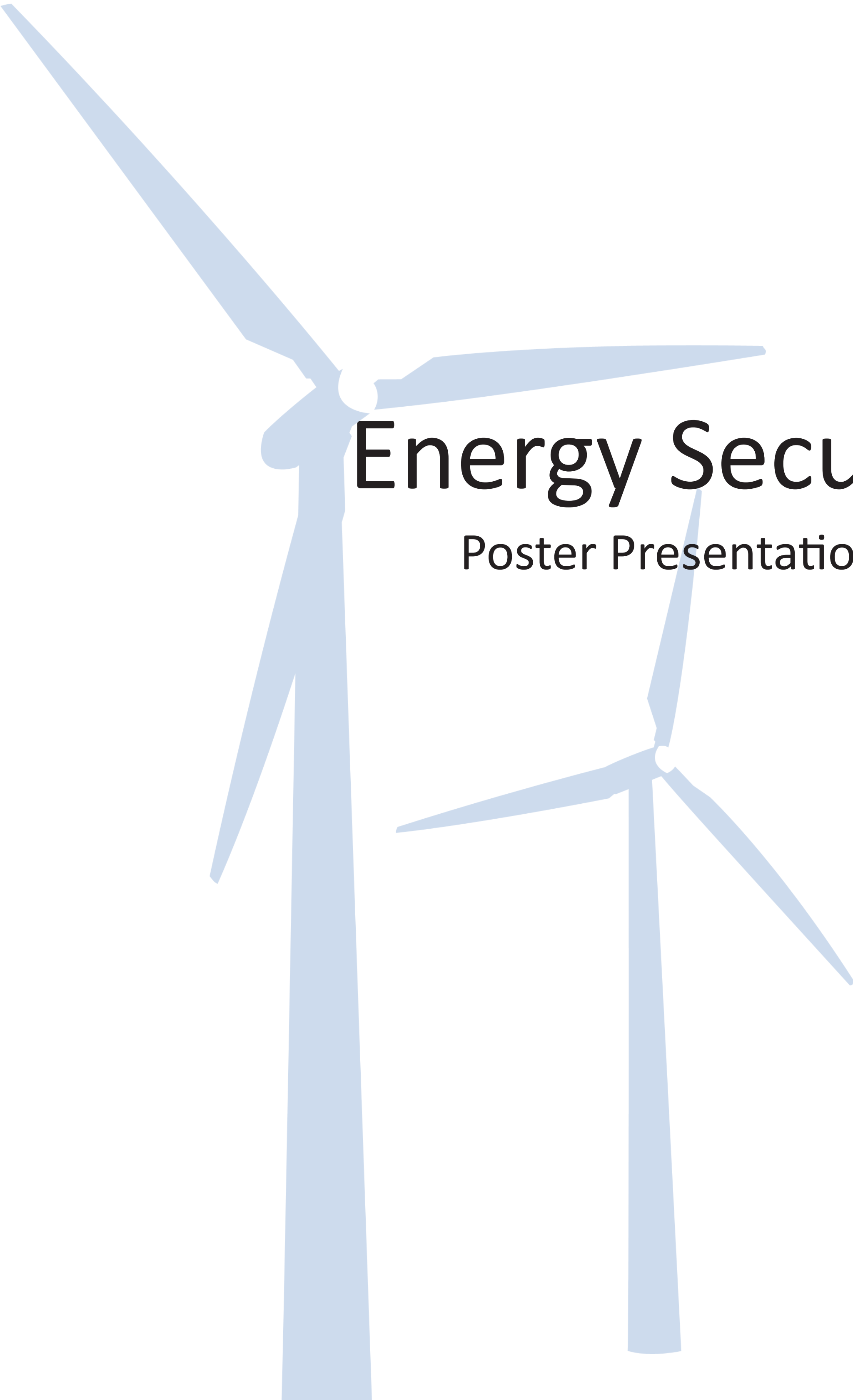
*Chief Scientist for International, Space, and Response*

*Los Alamos National Laboratory*

Herb Funsten received his Ph.D. from the University of Virginia in 1990, after which he became a postdoctoral researcher at Los Alamos.

Funsten served as director of the Laboratory's Center for Space Science and Exploration for six years and is currently the Chief Scientist for the International, Space, and Response (ISR) Division. He has led the development, launch, and operation of the National high energy neutral atom imager on NASA's Interstellar Boundary Explorer, the mass spectrometer on NASA's Radiation Belt Storm Probes mission, the plasma and mass spectrometers on DOE's SABRS payload and SABRS Validation Experiment payload.

Funsten is on instrument teams on NASA's TWINS, IMAGE, Cassini, and Mars Odyssey missions. He is an author of over 90 scientific papers in the refereed literature and 18 other publications spanning planetary science, space physics, and atomic physics. He has nine patents in mass spectrometry and detection technologies. He has served as a referee for 16 journals and has received two NASA Group Achievement Awards, two Los Alamos Distinguished Performance Awards, and LANL's 2009 Women's Career Development Mentoring Award.



# Energy Security

## Poster Presentations

## Novel Engineering Solutions to Make Wind Power Viable (Poster 1)

Curtt Ammerman (Principal Investigator), G. Park, R. Linn, B. Balasubramanium, and K. Farinholt

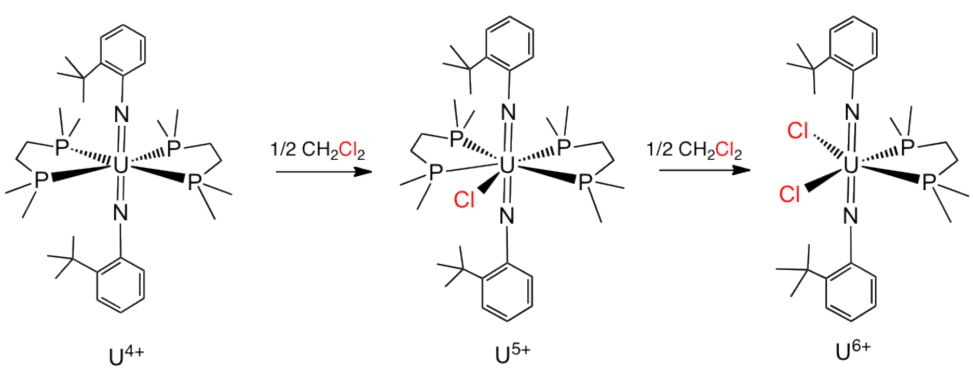
There are enough wind resources in the US to provide 10 times the electric power we currently use, however wind power only accounts for 2% of our total electricity production. One of the main limitations to wind use is cost. Wind power currently costs 5-to-8 cents per kilowatt-hour, which is more than twice the cost of electricity generated by burning coal. Our Intelligent Wind Turbine LDRD Project is applying LANL's leading-edge engineering expertise in modeling and simulation, experimental validation, and advanced sensing technologies to challenges faced in the design and operation of modern wind turbines.

*Advanced Damaged Detection Sensor Test on 9-Meter Blade at the National Renewable Energy Laboratory.*

## Fundamental Studies of the Oxidation of Uranium Compounds: Towards the Conversion of Carbon Dioxide to Fuels (Poster 2)

James Boncella (Principal Investigator), L. Spencer, R. Jilek, and B. Scott

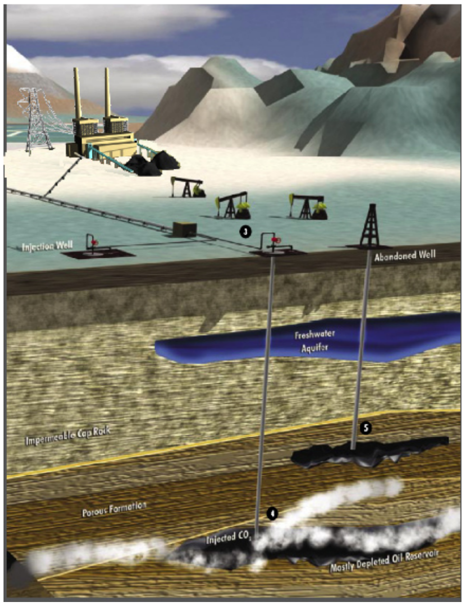
This project is focused on developing an understanding of the oxidation/reduction chemistry of uranium compounds. Ultimately, we are interested in determining if this metal can behave as a catalyst for chemical reactions such as the reduction of carbon dioxide into potential fuels and the reduction of water to give hydrogen gas. These important chemical reactions are simple, but involve the exchange of multiple electrons between reaction partners, which makes them difficult reactions that require metal catalysts that undergo similar redox transformations. We are investigating the interconversion of novel uranium compounds between the 4+, 5+ and 6+ oxidation states as a first step toward the larger goal of catalyzing the important reactions stated above.




*Oxidation of uranium complexes from the 4+ through 6+ oxidation states.*

## Reducing the Impact of Burning Fossil Fuel on Climate by Storage and Disposal of Carbon Dioxide ($CO_2$) in the Deep Subsurface (Poster 3)

Bill Carey (Principal Investigator), A. Abdel-Fattah, S. Backhaus, Q. Kang, P. Lichtner, D. Moulton, D. Newell, and Y. Zhao




Global warming induced by $CO_2$ emissions from coal-fired power plants, automobiles and other fossil fuels is an enormous scientific and political challenge. We are studying the feasibility of capturing $CO_2$ from power plants and injecting it into deep underground formations (such as sandstone). One simplified view of the process is that it involves withdrawing oil and gas and replacing it with $CO_2$. Through experiments and modeling, we are developing the scientific tools to design the injection process so that $CO_2$ is stored permanently and has little chance of leaking back to the surface.

*Schematic diagram illustrating the capture of $CO_2$ from a coal-fired power plant, transportation of the $CO_2$ by pipeline to an injection well, and injection of the $CO_2$ into the deep subsurface.*

## Greener Pastures Ahead: Environmentally Friendly Routes to Commodity Chemicals (Poster 4)

David T. Fox (Principal Investigator), K. Hotta, D. Edlin, J. Welsh, M. Waltman, G. Montano, and A. Koppisch


*Multiple examples of products currently consumed world-wide. The materials used to make these products are simple compounds called commodity chemicals. Green chemistry through bioengineering platforms will provide an alternate route to the identical chemicals.*

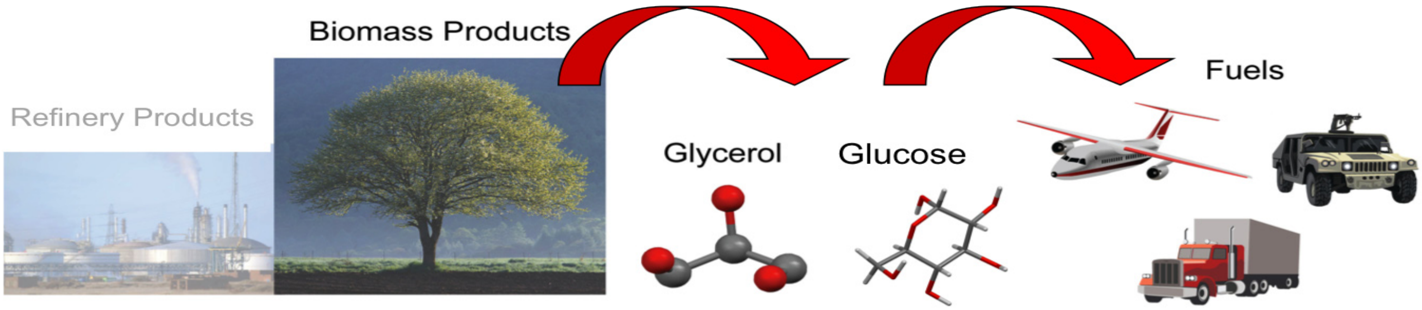
Current industrial methods to so-called “commodity chemicals” are almost completely based on fossil fuel conversion strategies. Some examples of commodity chemicals include the essential building blocks for the production of nylon, plastics, flavorings, and food preservatives, all of which are produced on a multi-billion ton scale/year. Continued consumption of irreplaceable fossil fuels, greenhouse gas production, and massive quantities of environmentally unfriendly waste generation will invariably destroy our precious earth. As such, we are bioengineering microbes to make the identical chemicals currently produced by industrial methods. We envision our approach will result in the following outcomes:

- Help alleviate our dependence on fossil fuels
- Reduce greenhouse gases (GHG) worldwide
- Lower energy consumption and project costs
- Be more environmentally responsible and profitable

## The Efficient Conversion of Non-Food Based Biomass into Fuels (Poster 5)

R. Baker, E. Batista, W. Chen, R. Currier, M. Dirmyer, and J. Gordon (Principal Investigator)

Within the next 30 years, world energy consumption is projected to double. It is essential to our National security that renewable alternatives to petrochemical feedstocks for hydrocarbon fuels are developed. A reliable supply of these fuels would ensure that the transportation of food, medicine, and consumer goods about the country remains uninterrupted, regardless of sociopolitical conflict. The development of alternative energy sources is thus increasingly urgent, particularly in light of escalating $CO_2$ emissions and concern over global warming. In this regard, *non-food* derived biomass represents an attractive energy source, being both renewable and carbon-neutral.




*The goal of this project is to lessen our dependence on refinery based sources and move towards upgrading of biorenewable sources for transportation fuels.*

## Genomic Characterization of Environmental Microbal Communities (Poster 6)

Nick Hengartner (Principal Investigator)

Microbial communities are complex "supra-organisms" of bacteria, archaea, single-cell eukaryotes and viruses that function together as a whole in order to survive and thrive in their natural environmental niches. Microbes make up the majority of the living biomass on Earth and as such, are major contributors to carbon cycling and to the biogenic production and destruction of other greenhouse gases, including N2O and methane. Our present lack of understanding regarding the biochemical fluxes of C and N within these microbial communities constitutes a major source of uncertainty in our predictions of the consequences of climate change and human activity such as fossil energy use.

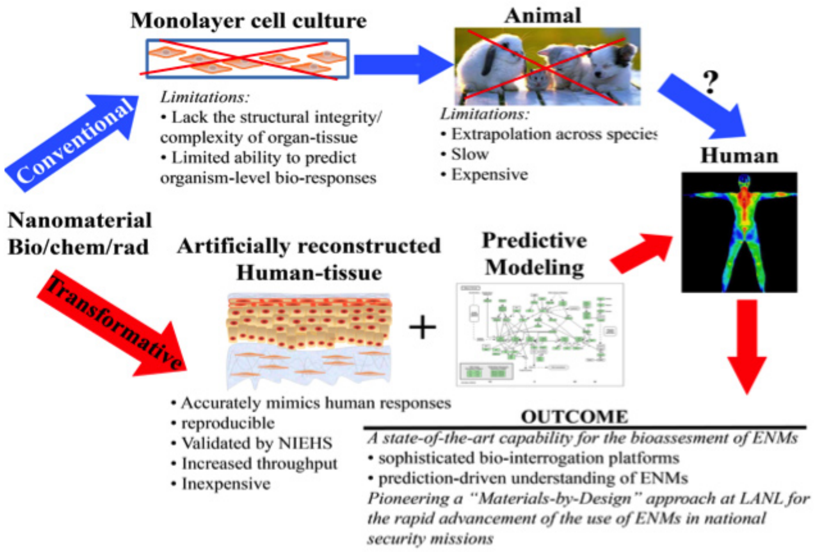
Characterizing the genomic potential of microbial communities, a nascent field known as metagenomics, can help bridge this information gap by revealing how climate change impacts the broad composition and function of members within bacterial communities, and by quantifying the net effect of these changes on both the C and N cycles. Effectively characterizing the genomic potential of microbial communities is challenging. In part due to the intrinsic interdependencies within microbial communities, only a small fraction (<1%) of all bacteria have been cultivated in isolation, a pre-requisite for standard genome sequencing efforts.

Shotgun sequencing of environmental samples is possible, but its usefulness is limited by our ability to analyze the data composed of short fragments of DNA, called reads. Combining our understanding of evolution with the knowledge of existing fully sequenced bacterial genomes, we have developed a novel tool that can assign phylogeny and function to many of the individual reads to determine who is doing what in the microbial community. And we can do this within a few hours on a desktop computer, making possible near real time analysis. Using this tool, we have the opportunity to start answering questions about how microbial ecosystems respond to climate change.

## Impact of Engineered Nanomaterials on Human Health  (Poster 7)

Rashi Iyer (Principal Investigator), J. Gao, and J. Hollingsworth

The intense interest in engineered nanomaterials (ENMs) is fueling a $1B industry that is expected to reach $1 trillion by 2015. This rapid pace of engineered nanomaterials development is outpacing our ability to understand their biological impact. Conventional bioassessment approaches used to assess engineered nanomaterials on a particle-by-particle basis is inadequate for providing a timely and accurate assessment of nanoscale-properties-dependent bioimpact. The goal of the proposed initiative is to develop a framework for the rapid and high-throughput assessment of the properties-dependent bioimpact of engineered nanomaterials.

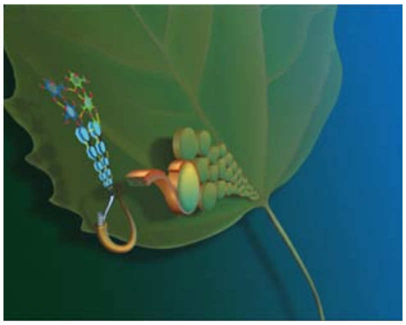



*Transformative bioassessment of engineered nanaomaterials*

## Making Fuels from Plants  (Poster 8)

Paul Langan (Principal Investigator), A. Asztalos, G. Bellesia, and A. Bradbury

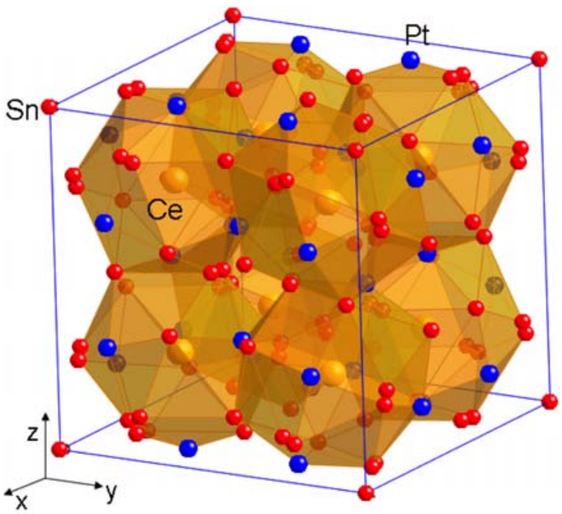
Cellulosic biomass, the fibrous material found in plants, is a potential clean and renewable, non-food feedstock for future biorefineries. Using biomass for energy is not a new thing. Wood burning fires have supplied heat, and sugar and starch containing crops such as sugarcane, grain, and corn have been used to produce ethanol fuel, throughout history. Early motor vehicles were designed to run on ethanol, and today around half of all transportation fuels in the US are blended with bioethanol derived from corn. Transportation fuels are also being blended with biodiesel from soybean and other vegetable oils. However, these crops are also sources of food and their diversion to fuel production can have undesirable consequences. Los Alamos scientists are developing breakthrough technologies to use a huge untapped reservoir of energy called cellulosic biomass. The challenge is to discover efficient ways of converting biomass into liquid fuels that will secure a sustainable energy future for the Nation.



*Plants use the energy from sunlight to convert the green house gas, carbon dioxide, into high-energy sugar molecules. These sugars are ideal for fermenting into biofuels such as ethanol or butanol. However, in the plant cell wall, sugar is trapped in crystalline cellulose fibers that act like high strength reinforcing rods. Cellulose is biosynthesized by joining glucose sugar molecules into long polymer chains that assemble into crystalline rods. These rods are then sheathed in less ordered polymers called hemicellulose which are made mostly from the sugar xylose, and then encrusted with the entangled polymer called lignin, in a complex architecture that is difficult to disrupt and which give plants their structure.*

## How Magnetism is Suppressed in Metals: The Case of $Ce_4Pt_{12}Sn_{25}$ (Poster 9)

Roman Movshovich (Principal Investigator)



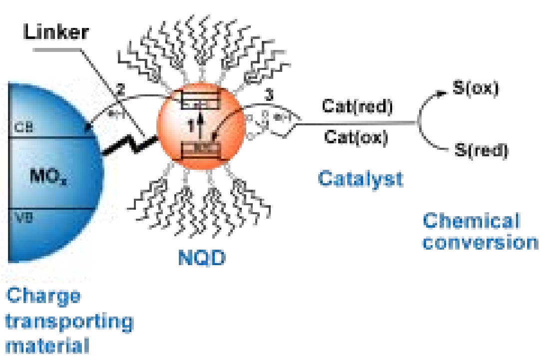

$Ce_4Pt_{12}Sn_{25}$ contains Ce – an element with electrons in an *f*-orbital far away from the nucleus, that behaves as a magnetic top – a spin. When ions with such *f*-electrons are close to each other, magnetic spins can order in magnetic structures, often with neighboring spin pointing in opposite direction to each other, i.e. antiferromagnetic (AFM) ground state. Conduction electrons, which are responsible for metallic properties, e.g. electrical conductivity, screen (reduce) magnetic field of *f*-electrons, by pointing their spins in opposite direction. $Ce_4Pt_{12}Sn_{25}$ reflects this competition between the screened and AFM states.

*Crystal structure of $Ce_4Pt_{12}In_{25}$.*

## Solar Energy Harvesting and Conversion Using Photocatalytic Nanomaterials (Poster 10)

Alexey Koposov, T. Cardolaccia, V. W. Manner, P. L. Szymanski, S. Kilina, E. Badeeva, V. Albert, S. Tretiak, T. J. Meyer, V. I. Klimov, and M. Sykora (Principal Investigator)

Development of new technologies for efficient harvesting and conversion of solar energy is a promising pathway to a long-term national energy security. Solar cells, devices converting solar energy directly to electricity, are one example of such technology. In our work we focus on development of an alternative approach, whereby captured solar energy is used to drive useful chemical reactions via process called photocatalysis. To maximize the efficiency of the photocatalytic solar energy conversion process we are exploiting unique properties of nanometer (10-9 meter) scale semiconductor materials also called nanocrystals quantum dots (NQDs).

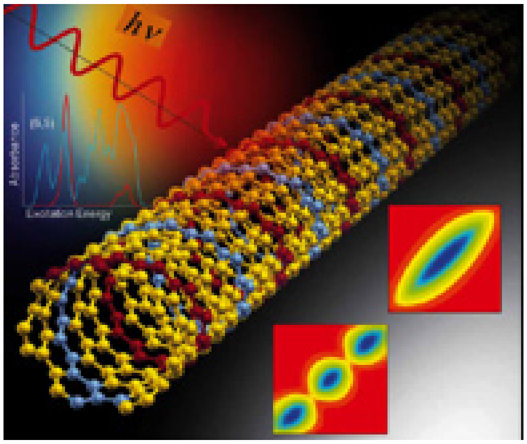



*Scheme showing the components and the principle of the operation of the photocatalytic material based on NQDs. Solar light absorption (1) is followed by electron transfer into charge transporting material (2) and from catalyst to NQD (3). The catalyst activated by the electron transfer process performs useful chemical conversion process.*

## Photodynamics and Photochemistry of Carbon Nanotube Materials (Poster 11)

Sergei Tretiak (Principal Investigator)

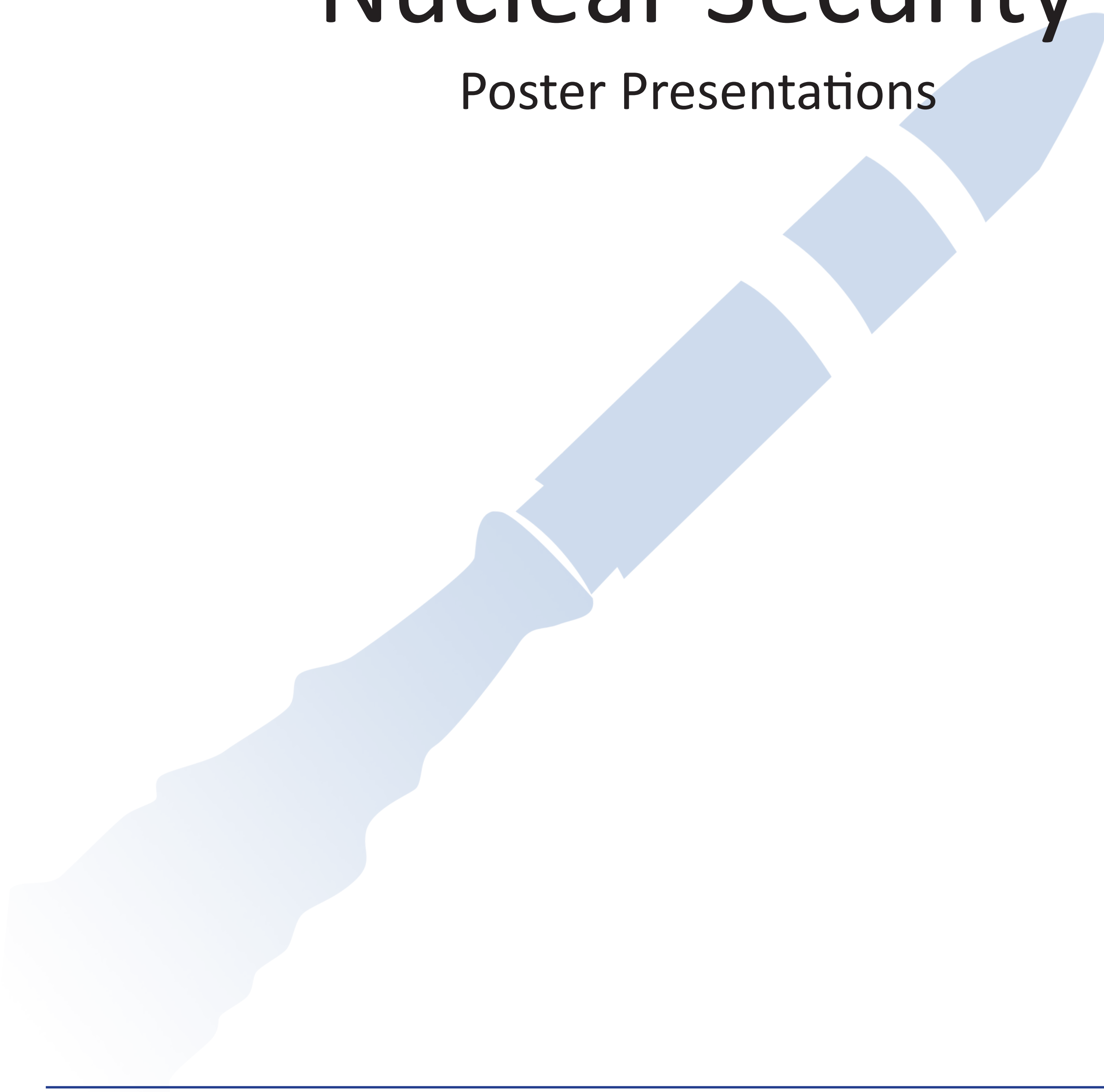
Carbon nanotubes constitute a class of the most promising technological high-strength materials with desirable and tunable electrical properties. Carbon nanotube and graphene based electronics are rapidly becoming today's reality given the huge R&D effort in the industry. This creates a need for modeling and simulation effort to predict physical phenomena and deliver comprehensive theoretical framework of electronic structure and dynamics in carbon nanotubes. In this project, using our theoretical modeling, we intend to achieve a quantitative description and a fundamental understanding of electronic processes in nanotube materials, provide novel material design strategies, and suggest practical nanotube applications.




*Our theoretical study uncovers how light excites multiple excitonic states of carbon nanotubes (shown as the cover page of the international journal Physical Chemistry Chemical Physics).*

# Nuclear Security

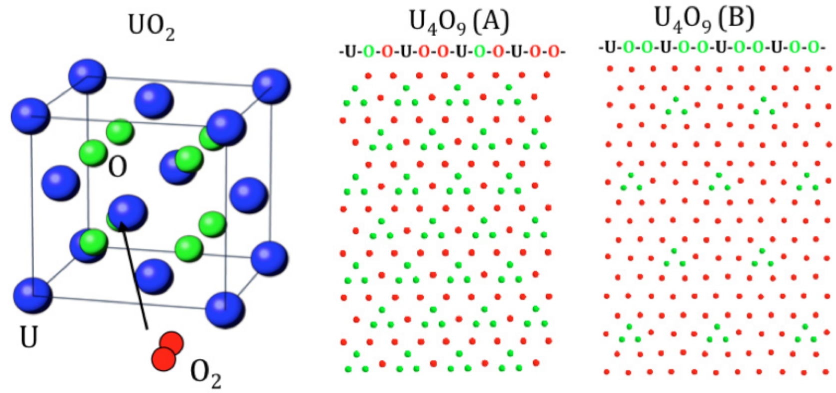
## Poster Presentations



## Triangular Atomic Patterns as Key to the Chemistry of Nuclear Fuels (Poster 12)

David Andersson, J. Lezama, C. Deo, B. Uberuaga, S. Conradson

Nuclear power plants produce electricity with very low carbon emissions and thus represent an opportunity to reduce the effects of global warming. Uranium dioxide, UO2, is typically the major constituent of current nuclear fuel. Understanding of its properties is essential for both nuclear power plant operations and for issues related to management of spent nuclear fuels. Here we illustrate how the use of advanced computer simulations enables us to identify triangular patterns of oxygen atoms in the structure of nuclear fuel materials (see figure) as key contributor to their chemical properties.

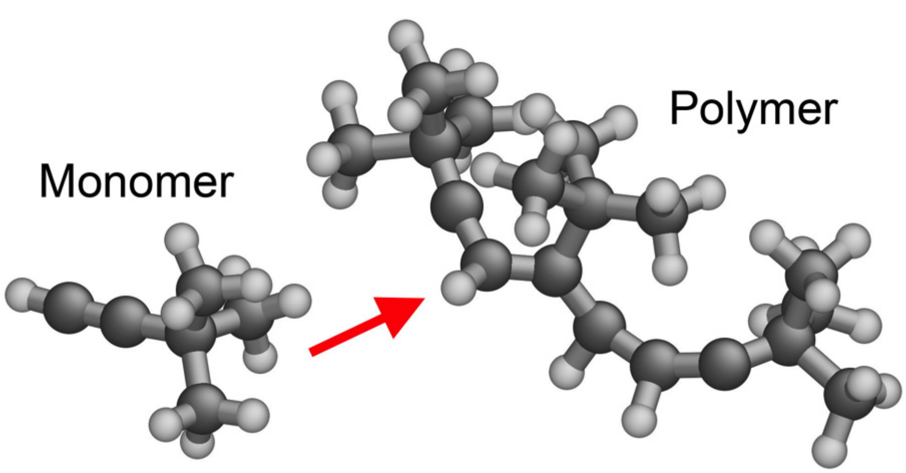



*In oxygen rich environments $UO_2$, which is the major component in today's nuclear fuels, takes up oxygen atoms and incorporate them into its lattice. These extra oxygen atoms form intriguing geometry patterns based on triangular clusters, as illustrated in the figures above, and many chemical properties of these materials can be understood from these characteristic patterns.*

## Resolving Shock-induced Chemical Reactions by Computer Simulation (Poster 13)

Edward Sanville, A. Niklasson, M. Cawkwell (Principal Investigator), D. Dattelbaum, and S. Sheffield

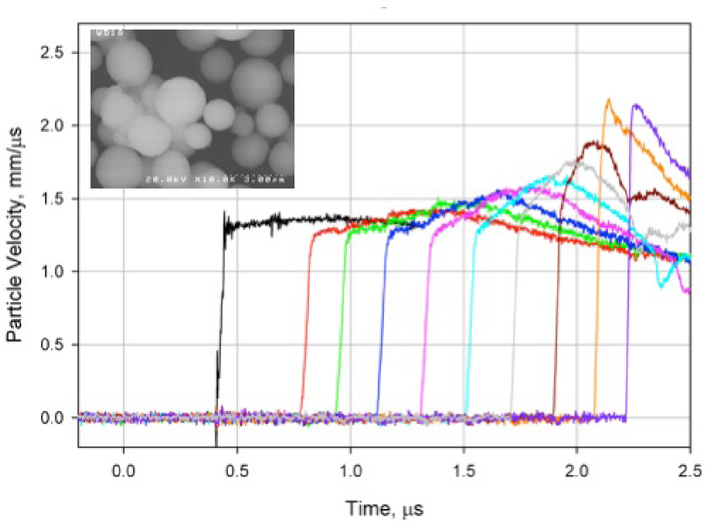
The shock compression of molecular materials leads to high temperatures and pressures that can induce chemical reactions by the making or breaking of covalent bonds. Sequences of reactions can occur over time scales so short that experiments struggle to resolve them. Computer simulations can track precisely the evolution of chemical reactions provided a suitable mathematical model of the bonding between atoms is available. We have developed and implemented a quantum description of bonding for organic molecules that is an optimal compromise between accuracy and computational speed, which we have applied very successfully in collaboration with experimental programs at LANL.




*Simulations of tert-butylacetylene molecules under thermodynamic conditions corresponding to those accessed in shock compression experiments revealed a radical chain polymerization reaction where individual molecules join together at the site of a carbon-carbon triple bond.*

## Understanding Explosives Initiation for Threat Evaluation and Mitigation (Poster 14)

D. Dattelbaum (Principal Investigator), S. Sheffield, R. Engelke, D. Stahl, and L. Gibson

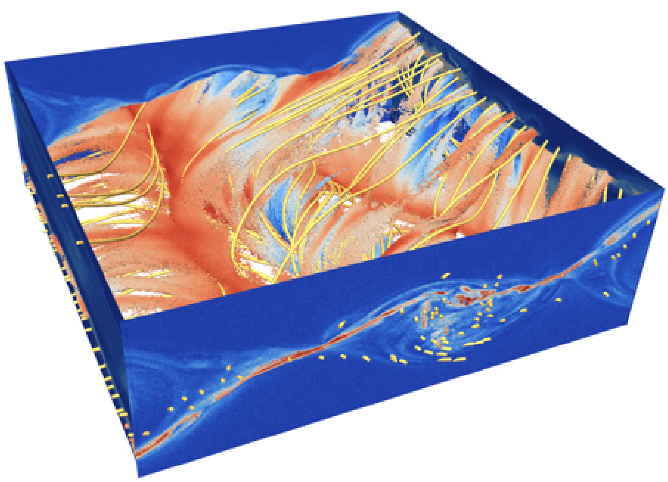



*The build-up from a shock to a detonation in nitromethane/ silica beads shocked to 7GPa.*

An improved understanding of how explosives initiate and detonate may enable science-based predictive capabilities of explosive response, and the design of better mitigation or defeat approaches. The initiation thresholds, mechanisms, and initiation pressure dependencies of relevant explosive formulations are being determined using in-situ measurements of shock and reactive wave profiles under controlled shock compression conditions. Liquid (or homogeneous) explosives display different initiation behaviors compared with multi-component (heterogeneous) explosive mixtures. Homogeneous explosives initiate via thermal explosion derived from bulk shock heating, whereas initiation in heterogeneous explosives is driven by the creation of localized regions of high temperature and pressure known as “hot spots.” We have established the initiation behaviors of several important liquid explosives, providing a comparison of their relative sensitivities, and revealing that the pressure dependencies of their run-distances-to-detonation appear to be similar across the series. Further, we have shown that the incorporation of hot spot “seeds” into liquid explosives are sensitizing, and we are isolating the key features of hot spots influencing initiation (critical sizes, separations, etc.). The relative effectiveness of solid vs. hollow particles in creating hot spots has been evaluated, and we have discovered that a balance exists between hot spot- and thermal –driven burn mechanisms. By studying explosives under controlled shock conditions, we are establishing a foundational knowledge regarding the important features that dictate initiation behaviors. Predictive models, derived from this knowledge, will be used to create the next-generation of explosive modeling capabilities for the Nation.

## Understanding Magnetic Storms in Space (Poster 15)

William Daughton, V. Roytershteyn, L. Yin (Principal Investigator), B. Albright, B. Bergen, and K. Bowers



Above the Earth’s atmosphere, there are violent storms driven by an unusual source of energy - the magnetic fields within hot ionized gases known as plasmas. These storms give rise to an explosive release of energy through a process called magnetic reconnection. Scientists believe this same process occurs in a wide range of different problems, including solar eruptions in the atmosphere of our Sun and within laboratory experiments where researchers are trying to confine plasmas with magnetic bottles to produce energy. Researchers at Los Alamos are using the most powerful supercomputers in the world in order to understand how this process really works.

*Simulation of magnetic reconnection performed on the Roadrunner supercomputer at Los Alamos. Shown is the 3D structure of the current density and magnetic field.*

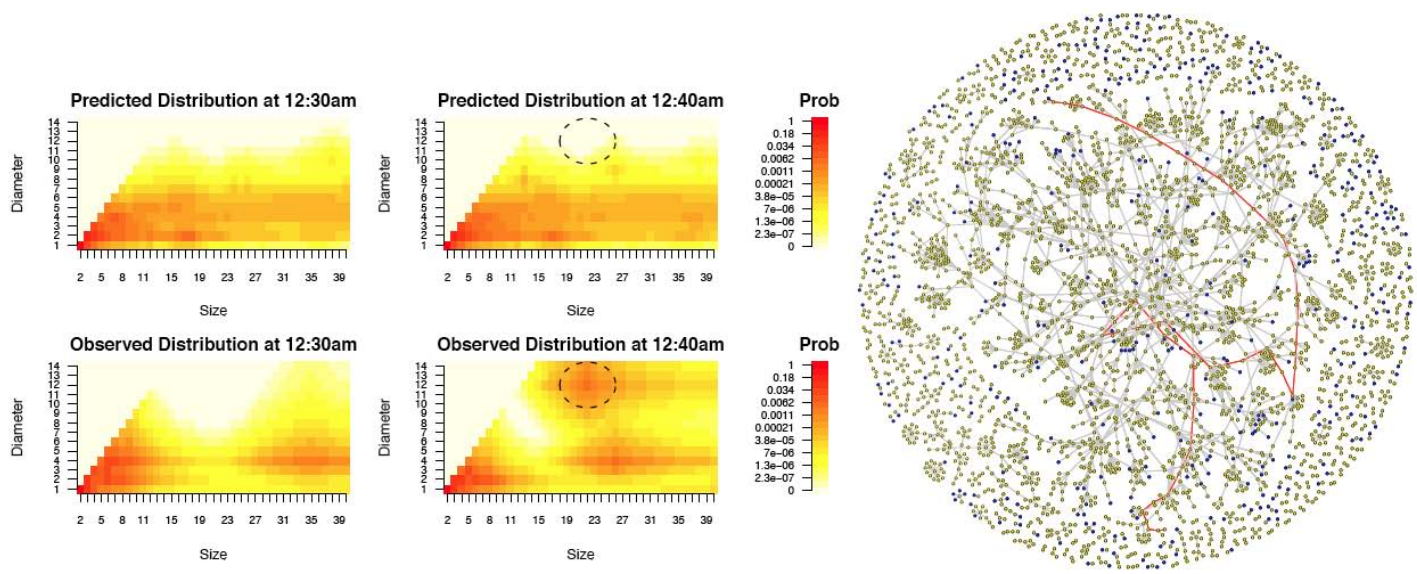
## Network-scale Analysis and Defense for Cyber Systems (Poster 16)

Mike Fisk (Principal Investigator), C. Storlie, G. Sandine, J. Neil, A. Hagberg, S. Vander Wiel, S. Eidenbenz, G. Yan, H. Djidjev, and M. Warren

Today's cyber attackers succeed by exploiting trust relationships between computers in ways that cannot be detected with current methods. We are developing new graph-based anomaly detection methods to identify these attacks. Traditional anomaly detection focuses on aggregate traffic at central nodes or on user-level monitoring. We are expanding anomaly detection methods to include the temporal nature of communications on cyber networks. This approach contrasts with the bulk of modern network and graph analysis work, which focuses on static graphs and graph evolution. This new area of graph anomaly detection will enable us to detect these modern attacks.

In this vein, two main contributions have been made by the LDRD team. First, we have derived several graph-based cyber data streams, including size and diameter distributions for graph components and/or graphlets of a dynamic network. We then developed novel statistical methodology to adaptively model these multivariate distributions over time. We can then compare the observed distribution to that which we were expecting under the model using relative entropy. The figure below indicates the utility of this approach for detecting anomalies in the evolution of LANL's ssh network.

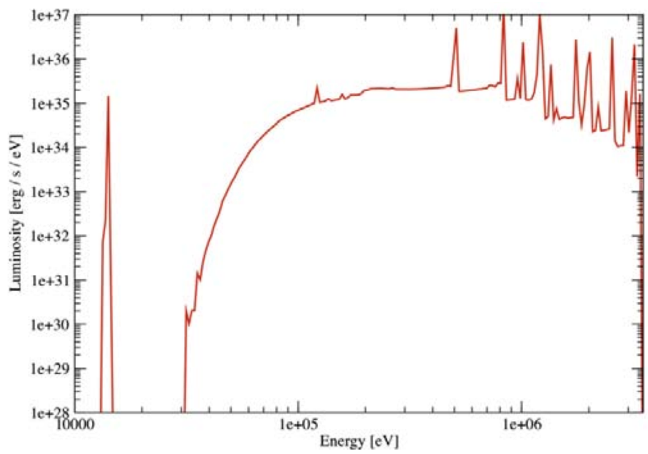
In addition, we have developed a method for detecting anomalous time-series patterns in paths in a graph. This detection proceeds as follows. First, we build a stochastic model of the data in each edge in the graph. This data is in the form of a sequence of counts of network activity on that edge. Next, new data is windowed in time, and a test is performed to determine how likely it is that we the new data arose from the learned model on the edge. Edges are glued together to form paths, and the overall anomalousness of the path can be determined.




*Multivariate Graph Anomaly Detection and Anomalous Diameter Plot*

## Understanding the Outbursts from Thermonuclear Supernovae (Poster 17)

James Colgan, C. Fontes, C. Fryer, A. Hungerford, S. Reddy (Principal Investigator), and H. Tierney



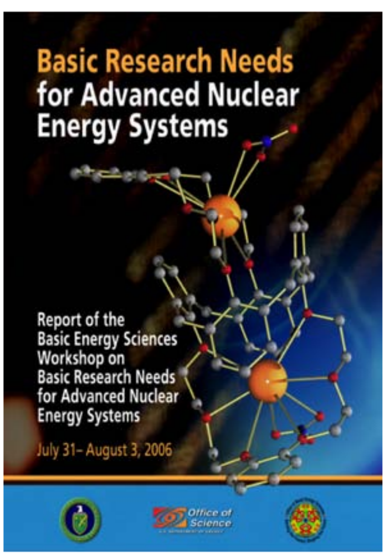

Supernovae are among the most energetic explosions in the universe. Thermonuclear supernovae occur when a compact star (aka white dwarf) fuses the carbon and oxygen in its core to drive a fusion bomb of astrophysical proportions. Supernovae are the production sites of nearly all the heavy elements in the universe (for example, thermonuclear supernovae produce the iron that make up most of the Earth's core) and are also powerful probes of the early universe. In this project, we study the observational outbursts of these supernovae from the infra-red up through X-rays and gamma-rays.

*Emission of gamma-rays as a function of the gamma-ray energy of from a thermonuclear supernova 60 days after the explosion.*

## Towards a Predictive Electronic Structure Capability for Strongly Correlated Materials (Poster 18)

Richard Martin (Principal Investigator), E. R. Batista, and E. Bauer

The motions of the electrons in a material dictate, either directly or indirectly, nearly all its physical properties. Electrons in carbon atoms are responsible for the chemical reactions that govern life; electrons in steel for its strength; electrons in copper for its electrical conductivity, and electrons in insulators such as the metal oxides for their resistance to electrical flow. The laws governing this motion are given by quantum mechanics, only the details differ from one material to the next, but those details make proteins different from superconductors!



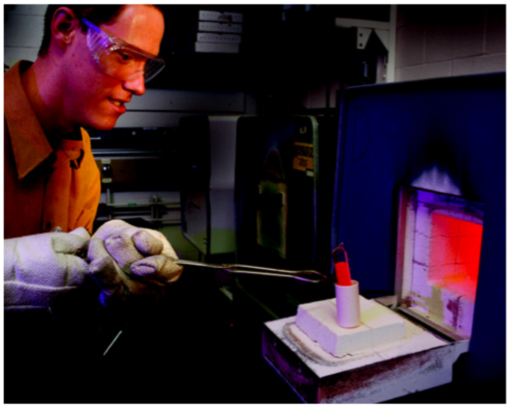

Today, we can model the motion of these electrons in molecules and solids and predict many of their properties using density functional theory. An era of experimental/computational codesign of new materials with prescribed properties is just now beginning. There is one important class of materials, however, for which the density functional theory fails completely. These 'strongly correlated' materials include the high-temperature superconductors, the collossal magneto-resistance oxides used in memory devices, the actinide oxides used in nuclear reactor fuel cycles, and the 'heavy electron' compounds. 'Heavy' refers to their electrical properties; their electrons neither move freely like good conductors, nor are they stationary, localized on a single atom, like insulators. They move, but sluggishly -- they are 'heavy.'

We will describe a joint experimental/theoretical program whose goal it is to understand and predict the properties of these materials. Together, we hope to generate a theory that brings these materials into the realm of those whose properties may be predicted by computation.

*"The scientific challenge is to develop a well-formulated and predictive first-principle theory for relativistic correlated f-electron materials and complexes."*

## The Seaborg Institute Postdoc Program (Poster 19)

Albert Migliori (Principal Investigator and Deputy Director)



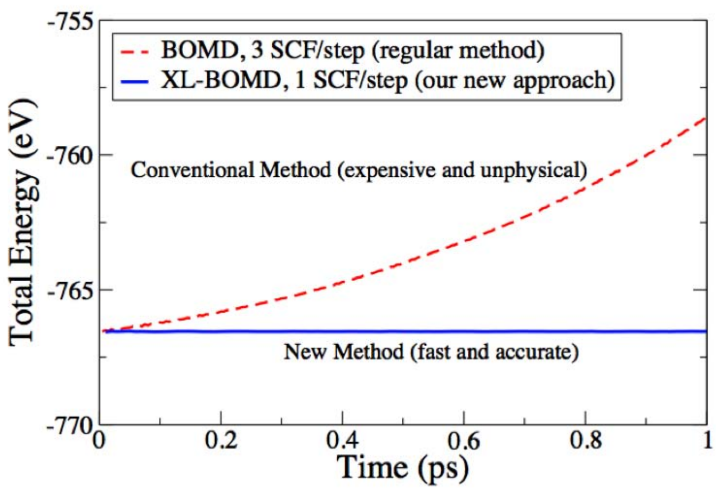
Knowledge of actinide science continues to be essential to the US and central to the mission of the NNSA, including national defense, energy, environmental restoration, and radioactive waste management. With nuclear weapons technology continuing to play a key role in defense policy for the foreseeable future, knowledge and expertise in the production, processing, purification, characterization, analysis, and disposal of actinide elements is essential to US national security. The purpose of the Seaborg Institute Postdoctoral Fellows Program is to foster sustained excellence and enhanced external visibility in actinide science; to establish a broad intellectual community for actinide science in support of Laboratory missions; and to provide a mechanism to attract and retain a future generation in actinide scientists and engineers.

*Former Seaborg postdoc Eric Bauer readies a polycrystalline sample for annealing in a study of superconductivity in a plutonium compound. Bauer is now a staff member in Materials Physics and Applications (MPA) Division.*

## First Principles Molecular Dynamics for Extended Length and Time Scales (Poster 20)

Edward Sanville, A. Niklasson (Principal Investigator), M. Cawkwell, D. Dattelbaum, and S. Sheffield

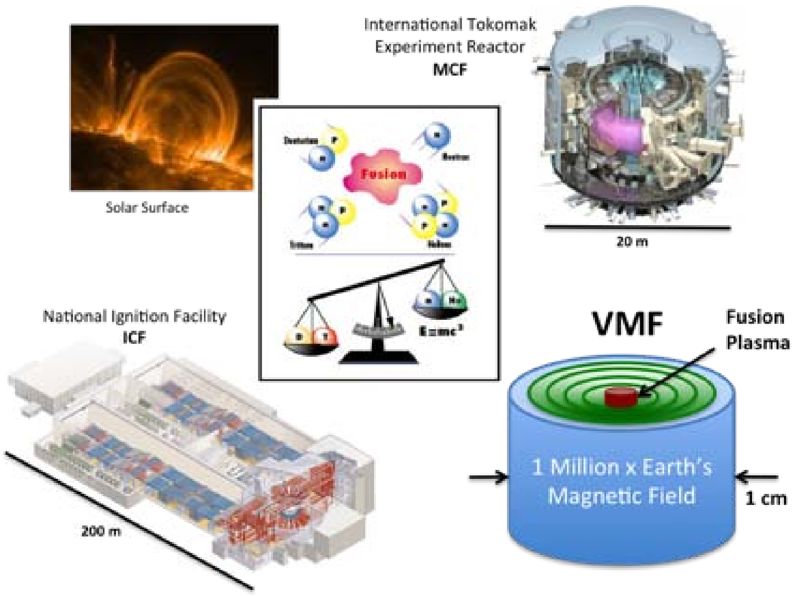
The ability to analyze and experiement with materials directly on a computer without any experimental input is rapidly transforming materials science, chemistry and molecular biology. Molecular dynamics simulations allow detailed studies of fundamental material properties such as phase transitions, chemical reactions and molecular structures. Molecular dynamics simulations, where the molecular motion is derived directly from the first principles of quantum mechanics is currently the most accurate ``gold'' standard for atomistic simulations. First principles simulations are possible without any input from experiments and therefore allow for analysis and predictions of material properties under conditions that not naturally can be achieved under laboratory conditions or to a fraction of the experimental cost. The simulations also give a more complete and detailed description that enables an understanding and sometimes prediction of materials with new tailored properties that often is very difficult, time consuming, or expensive to achieve through experiments. Unfortunately, current first principles molecular dynamics simulations are limited by some fundamental shortcomings such as a very high computational cost for large systems and unbalanced unphysical molecular trajectories with a systematic long-term energy drift, i.e. the system is artificially heated up or cooled down. Accurate atomistic simulations for extended length and time scales, which is absolutely pivotal for many problems of interest, are therefore currently not achievable. I will present the outcome of our attempts to reach this goal. The key result of our exploratory research is a novel, but surprisingly simple, theoretical framework for a new generation of first principles molecular dynamics that overcomes fundamental problems that so far has hampered accurate simulations for extended length and time scales




*The figure shows the accurate and physically correct energy conservation that is achieved with our new method (XL-BOMD) at a third of the computational cost for a regular simulation (BOMD).*

## Velocity Multiplication for Thermonuclear Fusion (Poster 21)

Christopher Rousculp, R. Watt (Principal Investigator), and A. Sgro




There are three traditional methods for producing nuclear fusion, two are man-made.

Solar Fusion – The sun's gravity holds together a very large plasma (1025 m3).

Magnetic Confinement Fusion (MCF) - A magnetic field, 1 million times the earth's, confines a large plasma (~103 m3) inside a donut shaped tokomak.

Inertial Confinement Fusion (ICF) – Hundreds of lasers are used to confine a very small amount of plasma (<1 cm3).

Both of the earthly ventures are very large-scale, complex projects. Our idea is to combine aspects of both and develop a small-scale, simpler, inexpensive platform to study nuclear fusion.

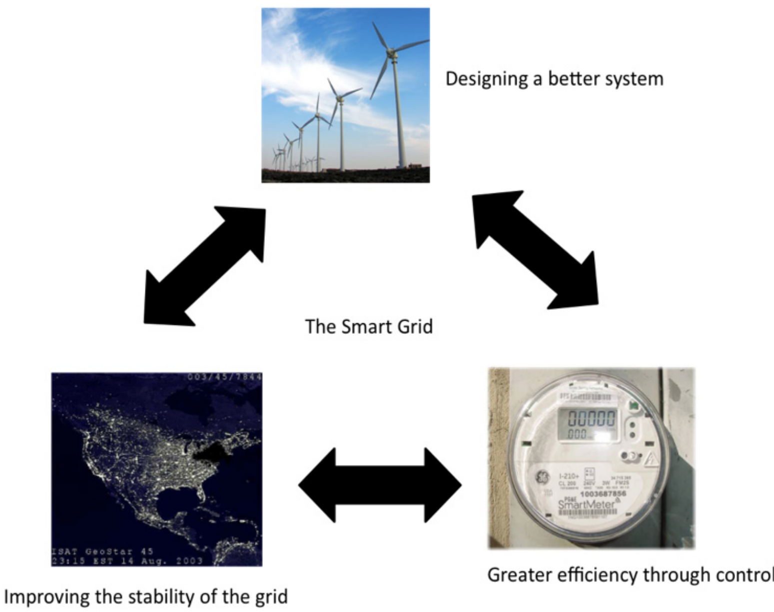
In velocity multiplication fustion (VMF), a strong magnetic field propels a set of metal cylinders to very high velocities via multiple collisions with each other. The innermost cylinder, traveling at 20 times the speed of a bullet, confines a small plasma to create nuclear fusion for scientific study.

# Global Security

## Poster Presentations

## The Smart Grid: Designing, Controlling and Analyzing the 21$^{st}$ Century Electric Power Grid (Poster 22)

Michael Chertkov (Principal Investigator), and R. Bent

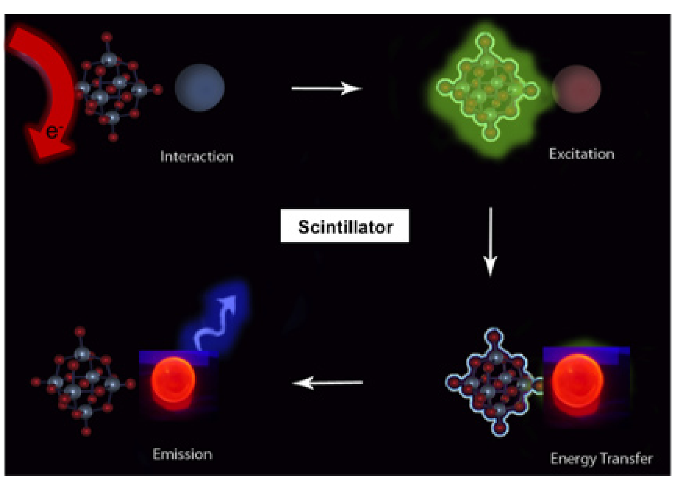



*The three pillars of LANL's smart grid project.*

The 21$^{st}$ century electric power grid is experiencing a rise in the insertion of new technologies (i.e. wind and solar power generation, hybrid electric vehicles, computerized sensors, and smart meters). These technologies pose a number of complex challenges including how to best upgrade the existing grid to accommodate these technologies, how to use the technologies to better control the daily operations of the system, how to mitigate intermittent effects associated with renewable generation, and how to exploit new information about the status of the system to improve stability and reduce the occurrence of black outs. This project seeks to address these challenges through sophisticated techniques from power engineering, optimization and control theory, computer science, information theory and statistics.

## Novel Materials for Detection of Radioactive Materials (Poster 23)

Rico Del Sesto (Principal Investigator), D. Ortiz-Acosta, and R. Feller



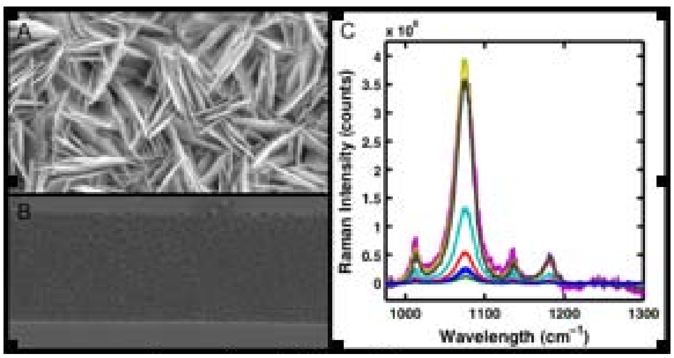

*Designing materials to detect radiation through light-emission.*

Understanding how scintillators work is necessary for the enhanced detection and non-proliferation of radioactive materials for global security. Through a combined approach of materials synthesis and theoretical modeling, we aim to design new, more efficient optical materials and model their luminescent behavior. The synthesis of modular molecular and supramolecular materials containing phosphors allows us to control the size and dimensionality of such materials and provides us with new insights into the scintillation process. The understanding of how molecular phosphor materials work through synthesis, characterization, and theoretical modeling provides a platform for the design of more efficient detector materials.

## Designer Nano-Architectures for Advanced Analyte Detection (Poster 24)

Nathan Mack, C. Brady, L. Brown, P. Xu, S. Jeon, H. Wang, and S. Doorn (Principal Investigator)

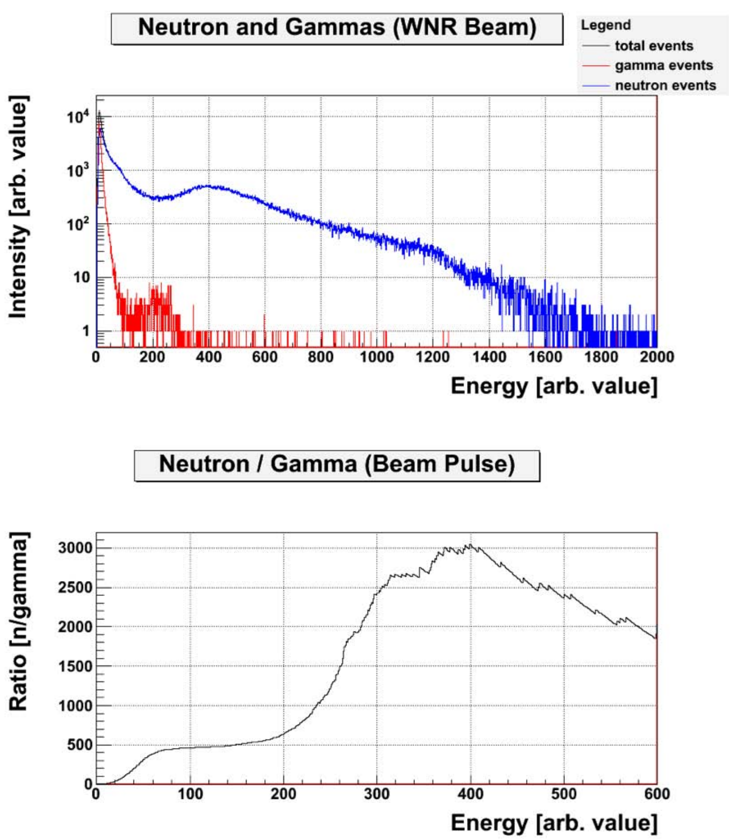
Detection and identification of chemical and biological compounds at extremely dilute concentrations is an ongoing and formidable objective for national security and threat reduction missions. Spectroscopic analysis methods such as Surface Enhanced Raman Spectroscopy (SERS) are capable of being greatly enhanced when using appropriately designed metal nanomaterials. This work seeks to control and manipulate metallic nanoparticles through synthetic and physical means in order to investigate the ideal aggregate size and geometry for maximum SERS excitation. Surface-based particle patterning techniques enable a combinatorial approach to assembling simple metallic particle aggregates in an effort to deduce ideal aggregate structures. These simple nanoparticle structures will provide insights towards more complex architectures, which will greatly improve SERS-based analyte detection.




*A) Silver nanostructures grown on polymer surfaces. B) Nanoparticles assembled into surface patterned wells. C) Representative Raman spectrum from a nanostructured surface.*

## A Novel Neutron Detector (Poster 25)

Ernst Esch (Principal Investigator), R. Muenchausen, S. Stange, I. May, F. Taw, and F. Tovesson



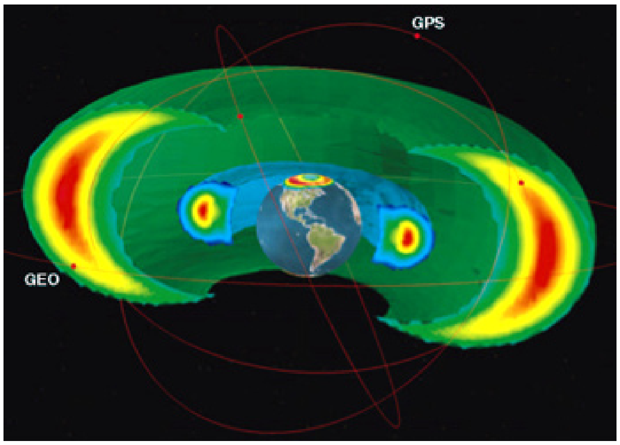

Neutron monitors are commonly used for a variety of nuclear physics applications. A scintillating neutron detector, consisting of a liquid scintillator loaded with fissionable material, has been developed, characterized, and tested in a neutron beam line, and shows a significant improvement in neutron sensitivity compared with a conventional fission chamber. Recent research indicates that it is possible to load nanoparticles of fissionable material into a scintillating matrix, with up to three orders of magnitude higher loading than typical fission chambers. This will result in a rugged, cost-efficient detector with high efficiency, and short signal rise time.

*Neuron and Gamma pulse ratios from preliminary data analysis.*

## Real-time Assimilative Radiation Belt Model (Poster 26)

Reiner Friedel, G. Reeves (Principal Investigator), M. Henderson, J. Koller, Y. Chen, J. St Leger, J. Holland, and S. Zaharia

An important part of Space Situational Awareness for national security assets is the exquisite knowledge of the energetic radiation environment at the spacecraft. This research combines point-measurements in space with a data-assimilative model (DREAM) to enable accurate estimates of the natural and artificial trapped energetic particle environment anywhere in geospace.



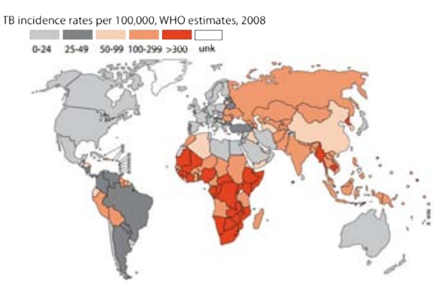

*Schematic of the earth's trapped high energy radiation belts. In red, an artificial HANE belt.*

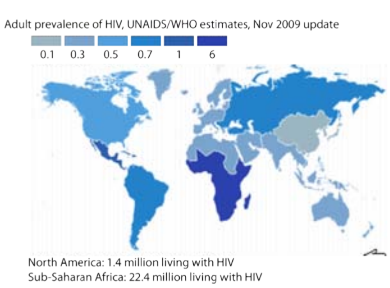
This model allows us to:

- Provide high-fidelity now-casts of the space environment based on a few existing key measurements.
- Estimate the space environment for space assets that do not carry environmental sensors – at a huge cost-saving compared to flying in-situ sensors.
- Provide a means of propagating artificially produced radiation belts (from HANE, high-altitude nuclear explosions) in time and space in the presence of the natural environment.
- The assimilative approach is an exiting research tool that allows us to test and improve the fidelity of the underlying physical models by providing quantitative data-based feedback.
- As the fidelity of the underlying physical models improves this model will be able to provide a predictive capability.

## Tracking the Emergence of Drug Resistance in HIV and TB (Poster 27)

Bette Korber (Principal Investigator), T. Bhattacharya, A. Chaudhary, W. Fischer, C. Gleansner, M. Goertz, K. Grace, and L. Green

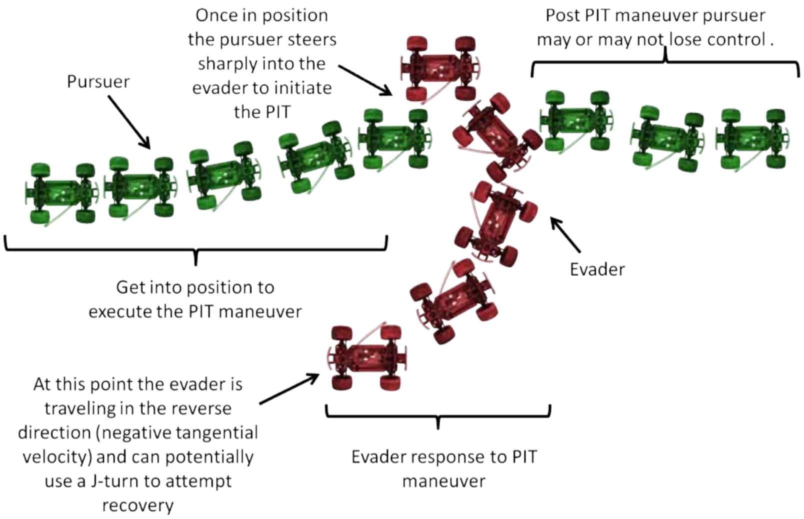



Mycobacterium tuberculosis, the bacteria that causes TB, has ravaged mankind for thousands of years and claims over 4000 lives worldwide every day. TB infections are increasing, particularly in Africa and Eastern Europe, and multidrug and extreme drug resistant forms of TB are on the rise. HIV/AIDS is estimated to infect 33 million people, with more than 2 million dying of AIDS each year. These pathogens have a terrible synergy, with co-infection leading to rapid demise and death, and fostering the spread of drug resistant TB. Better diagnostics and strategies for global tracking of drug resistance are urgently needed, at a moment in time when new DNA sequencing technology is revolutionizing capabilities for of pathogen diagnostics and surveillance. HIV is highly variable evolving rapidly even within patients, and the new technologies enable sequencing of tens of thousands of viruses from one individual. We have been developing computational strategies that allow evolutionary analysis of thousands of genetic sequences from a single individual. We have applied these methods to understanding the earliest immune escape events after infection with HIV, and showed that HIV undergoes a very rapid and extensive exploration of immune escape mutations during the first weeks of infection. In collaboration with colleagues in South Africa, we are tracking the emergence of HIV drug resistance in a prophylactic prevention study testing whether an anti-retroviral drug (Tenofovir) provided in a gel used during sex can block HIV transmission. Meanwhile our TB effort has resulted in developing highly sensitive assays for several TB biomarkers present in urine that correlate with progression to active disease. These biomarkers have potential diagnostic applications, and can be used to advance understanding the pathology of TB. We intend to bring these experimental advances together to study HIV-TB co-infection.

## Escape and Evasion by High-Speed, Autonomous Unmanned Ground Vehicles (Poster 28)

David Mascarenas (Postdoctoral Researcher), G. Park, and C. Farrar (Principal Investigator)



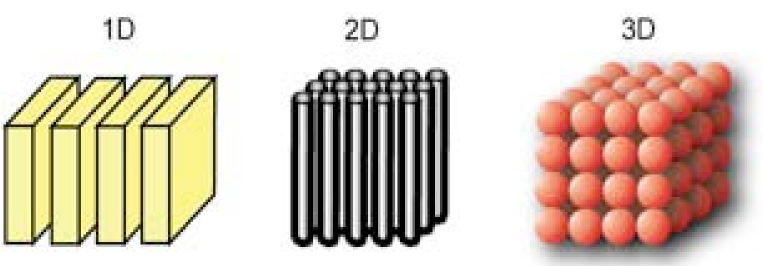

*Description of the Precision Immobilization Technique (PIT) being used for unmanned system escape and evasion research.*

Unmanned Ground Vehicles (UGV) are a mainstay for explosive ordinance disposal. Their role is expanding to include sentry duty, resource distribution, and casualty extraction. Warfighters have indicated that UGVs must be able to reliably traverse rough terrain at high speed to keep up with operations. Another obstacle to expanded use of UGVs in theater is the fear that UGVs will be captured and exploited by unfriendly forces. We need control policies that allow autonomous UGVs to quickly and reliably escape and evade hostile agents. Our initial work will consider the Precision Immobilization Technique (PIT maneuver) problem. The PIT maneuver is an attack strategy that could be used against autonomous convoys made up of car-like UGVs. Attacks might come from manned vehicles like motor scoters, or someday from enemy robots. A key challenge of this work will be to compute solutions fast enough for rapidly moving vehicles (think how fast a human driver has to react on the highway). Another major challenge is to combine information from a number of different sensors in near-real time.

## Terahertz Technology for Spectroscopy and Communications (Poster 29)

Nathan Moody (Principal Investigator), J. O'Hara, E. Simakov, and A. Taylor

The portion of the electromagnetic spectrum between microwaves and visible light, called Terahertz (THz), is considered a science frontier because its unique interaction with matter could help us better protect and understand the world around us. As a society, we utilize electromagnetic waves (e.g., light, microwaves, etc) routinely for everything from weapons and communications to cooking and manufacturing, but some frequencies, such as THz, are more difficult to generate and control. The IR/optical and microwave regimes have provided us with many important applications and the THz band may also yield unprecedented opportunities to interrogate, image, and uniquely identify unknown substances and structures. Due to inherently higher frequencies at THz, ultra high bandwidth communications channels could be constructed using THz sources and detectors which offer unique advantages over microwave links. The well established techniques for generating and controlling microwave and optical radiation have proven ineffective at THz frequencies, despite over a decade of intense effort. To utilize the THz part of the spectrum, our team has adopted a systematic approach to combine simulation, fabrication, and characterization of new classes of artificial media, whose unique structure provides a measure of control, generation, and detection of THz radiation. The form factors of these structures can be quite small, enabling eventual design of compact systems for a wide range of national security applications.

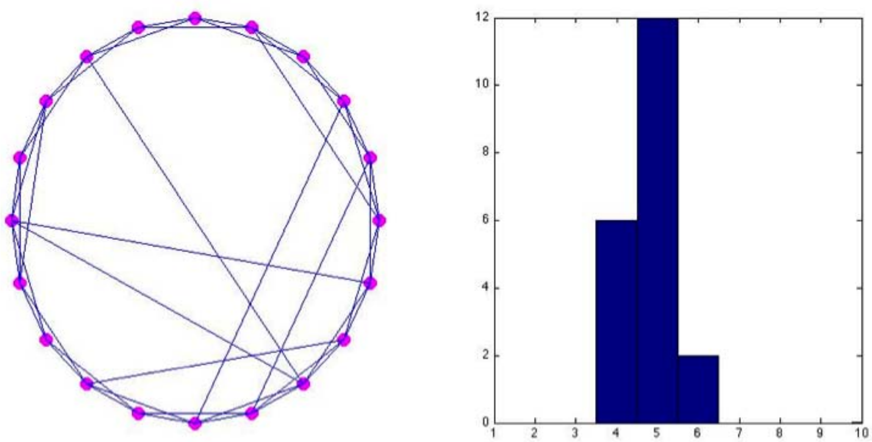



*New classes of engineered materials, such as these schematically shown 1D, 2D, and 3D structures (known as photonic band gap "crystals") are one example of artificial media with unique abilities to control the behavior of THz radiation.*

## How Does The Flu Get To You? (Poster 30)

Michael Murillo, L. Murillo, and A. Perelson (Principal Investigator)

Every winter many of us become ill with the influenza virus. Recent research suggests that the source of those viruses each year is South-east Asia. We are exploring how this disease moves within small communities (e.g., hospitals, prisons), cities, and across the globe. We have learned that a wide variety of tools and information are needed to grasp how influenza spreads. Armed with the necessary information and computational tools, we hope to contribute to our understanding of where flu comes from, how it spreads, where it goes, and why it does what it does. More importantly, this detailed understanding helps us to understand how we can save lives with the strategic use of intervention strategies.

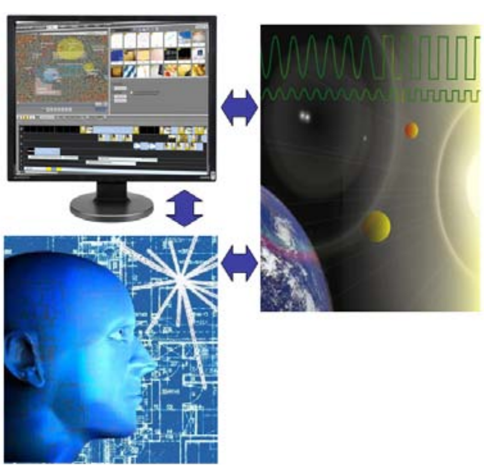



*Influenza moves through a community via a social contact structure. Here, we show a representation of the interactions of a group of twenty people (e.g., in a nursing home), as described with a "small-world" network model. The right panel shows the number of "friends" each person has in this particular community. How a disease spreads, and how it can be treated, depends on what this graph looks like.*

## Automated Image Analysis for Nonproliferation (Poster 31)

Reid Porter (Principal Investigator), L. Prasad, and J. Theiler

Thanks to decreasing costs of acquiring overhead airborne and spaceborne imagery, and to the increasing range of available image modalities (from video to hyperspectral), image analysts now have 1) the ability to see more of the world in more detail than ever before, and 2) more data than they can possibly look at. Because there are not enough trained human analysts, images are being left behind. One answer is to automate the image analysis: train computers do the job. But after half a century of energetic research on the topic, nobody really knows how to tell a computer how to figure out an image. Our best hope in the near term is data triage - concede that every image cannot be fully analyzed, but at least automate the identification of those images that are most desperately in need of an analyst's attention. This project has developed several new mathematical approaches to this problem, and demonstrated significant performance gains compared to the state-of-the-art. The project has prototyped image exploitation systems that leverage these new approaches in several application domains including remote sensing, and nuclear forensics.

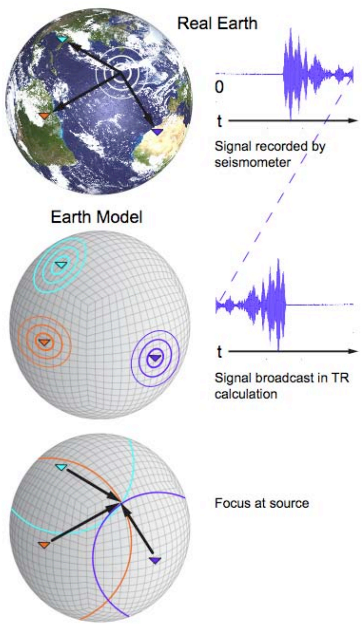


*Systems that can exploit the complementary strengths of humans and computers are critical to the efficient interpretation and monitoring of massive data streams produced by science and defense sensors.*

## New Seismic Techniques for Ground Based Nuclear Event Detection (Poster 32)

W. Scott. Phillips, P. Johnson (Principal Investigator), C. Larmat, and X. Yang

Ground-based nuclear event detection has been a national mission for decades, and has relied on cutting edge research by seismologists, acoustitians and radio chemists. The topic has attracted additional attention of late as our nation considers the Comprehensive Nuclear-Test-Ban Treaty (CTBT). Prior to the CTBT era, national interests dictated the monitoring of large nuclear explosions at a small number of test sites, using records collected globally, in keeping with the Threshold Test Ban treaty yield limit of 150 kT. In contrast, we now are required to detect nuclear explosions of any size over broad regions. The need to monitor small explosions has driven seismologists to develop new theory and methods to understand waves that have passed through highly heterogeneous crust and upper mantle of the earth. Exciting new techniques such as time reversal, and daylight imaging have found application to this new direction in explosion monitoring research, and have been nurtured by the LDRD program at Los Alamos. Our recent work has demonstrated the ability to study source radiation effects via time reversal, by feeding reversed seismic data into an earth model and allowing propagation back to their origin. We also apply related auto-correlation techniques to extract subtle signal delays in the scattered energy field that gives us event depth, a powerful event type discriminant, which is normally very difficult to determine. Finally, we will apply daylight imaging techniques to the natural noise field to enable detailed modeling of seismic wave speeds and attenuation characteristics in the shallow regions of the earth, which will allow us to isolate effects of the source, our ultimate interest.



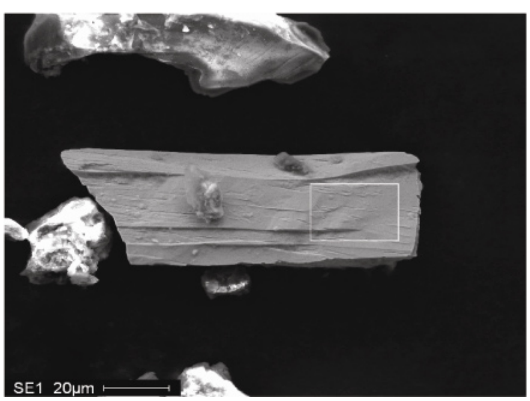

*Concept of time reversal. A reverse version of the wave propagation is created by re-broadcasting into a model the received signal but read backward-in-time.*

## Molecular Forensic Science of Nuclear Materials (Poster 33)

Marianne Wilkerson (Principal Investigator), A. Andersson, and J. Berg

Nuclear forensics is a broad term for analysis of intercepted nuclear materials to constrain or identify source, age, transport history, industrial material process, or intended use. Currently, nuclear forensic methods rely upon physical, isotopic, and elemental analyses using tools developed during the nuclear weapons era. Many signatures arising from production, conversion, and aging processes are chemical in nature, and spectroscopic measurements performed at LANL reveal the potential to detect persistent molecular signatures characteristic of material origin long after release.

Environmental studies by members of our team have shown the value of utilizing chemical signatures of actinide oxide materials to predict transport following release into the environment. Chemical speciation of actinide-oxide samples should also provide clues as to the age, source, process history, or transport of the material. The scientific challenge is to measure, identify and understand those aspects of actinide speciation that carry information about material origin and history relevant to forensics. Here, we will describe our efforts in material synthesis and analytical methods development to provide the fundamental science required to characterize actinide oxide molecular structures for forensics science.




*An X-ray fluorescence measurement confirms the presence of plutonium in material collected from contaminated soils at McGuire AFB, N.J. The Pu is likely an artifact of a fire at the site in 1960 that destroyed a Bomarc-A airframe.*

## Evolution and Function of Microbial Signatures (Poster 34)

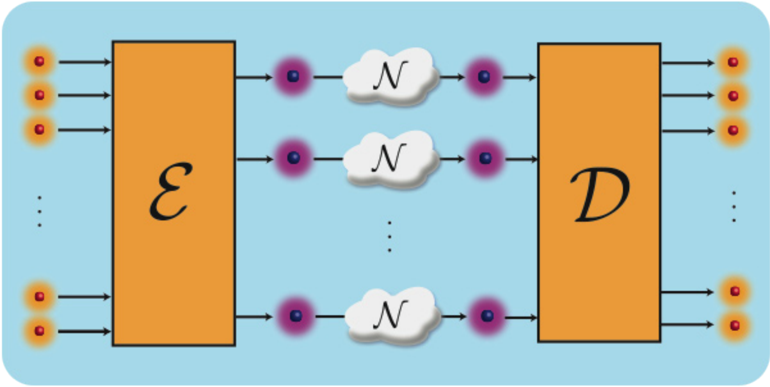
Murray Wolinsky (Principal Investigator) and C. Stubben

Microbial signatures are relatively short nucleic (or amino) acid sequences that can identify bacteria or viruses. Determining these signatures is vital for detecting biothreat agents, for microbial forensics, and for public health applications such as diagnostics. While considerable effort is currently expended on finding signatures, very little effort has been placed on understanding them. This research is an attempt to balance this situation by providing basic insights into the evolutionary and functional significance of microbial signatures. We have modeled the empirical distribution of signatures from thousands of microbial strains and identified critical features to target or avoid such as mobile regions characterized by frequent duplications. We have developed various techniques based on DNA thermodynamics and other methods to identify unique signatures at different nodes in a phylogenetic tree or among different phenotypic groups (e.g. between pathogens and non-pathogens), and then to relate the signatures back to a detailed set of genome annotations to identify the functional significance. A better understanding the evolutionary forces that determine these signatures and how they relate to biological function will enable future improvements in detection systems and public health diagnostics.

## Quantum Information Science (Poster 35)

Robert Ecke (Principal Investigator) and J. Yard (Postdoctoral Researcher)

The possibility of manipulating quantum states presents exciting scientific possibilities. Because quantum systems are hard to simulate on conventional computers, computers utilizing quantum coherence should be intrinsically more powerful than conventional ones. Noise is a challenging obstacle for quantum engineering, and fighting it requires a deeper understanding of the nature of information at the quantum level. What is quantum information? How can it be quantified and protected from noise? This project studies these and other related questions, finding that quantum information shares central features with conventional information, while differing in fundamental and interesting ways.

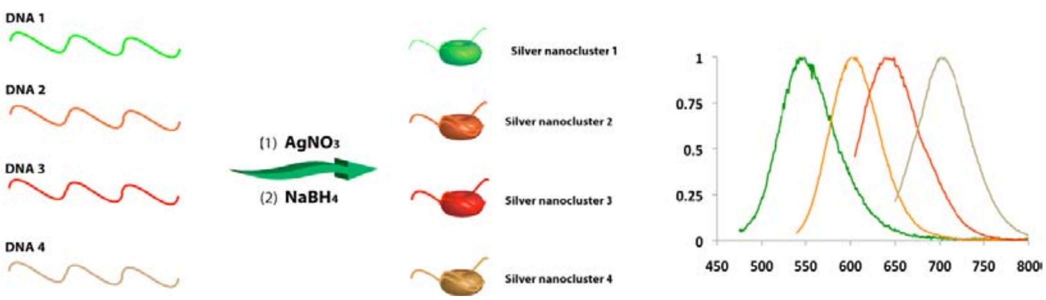



*Scheme for protecting the quantum state of a collection of quantum bits from noise through encoding and subsequent decoding.*

## Synthesis and Biosensing Applications of Noble Metal Nanoclusters (Poster 36)

Jaswinder Sharma (Postdoctoral Researcher), H. Yeh, J. Werner, and J. Martinez (Principal Investigator)

Oligonucleotide-templated silver nanoclusters, consisting of few atoms, have gained a substantial interest due to their unique fluorescence properties, and the potential applications of these nanoclusters for bio-and chemical-sensing, invivo imaging, and in-vitro bioassays. While many reports have been published demonstrating the use of oligonucleotides for synthesis of silver nanoclusters, synthesis of oligonucleotide-templated nanoclusters with tunable fluorescence emission is still in its infancy. Herein, we address both of these issues by synthesizing oligonucleotidetemplated silver nanoclusters with tunable emission, and using them in detection of specific biomolecules, without using stringent coupling conditions.




*Schematic showing the synthesis of silver nanoclusters emitting at different wavelengths.*

## Petascale Synthetic Visual Cognition: Large-scale, Real-time Models of Human Visual Cortex on the Roadrunner Supercomputer (Poster 37)

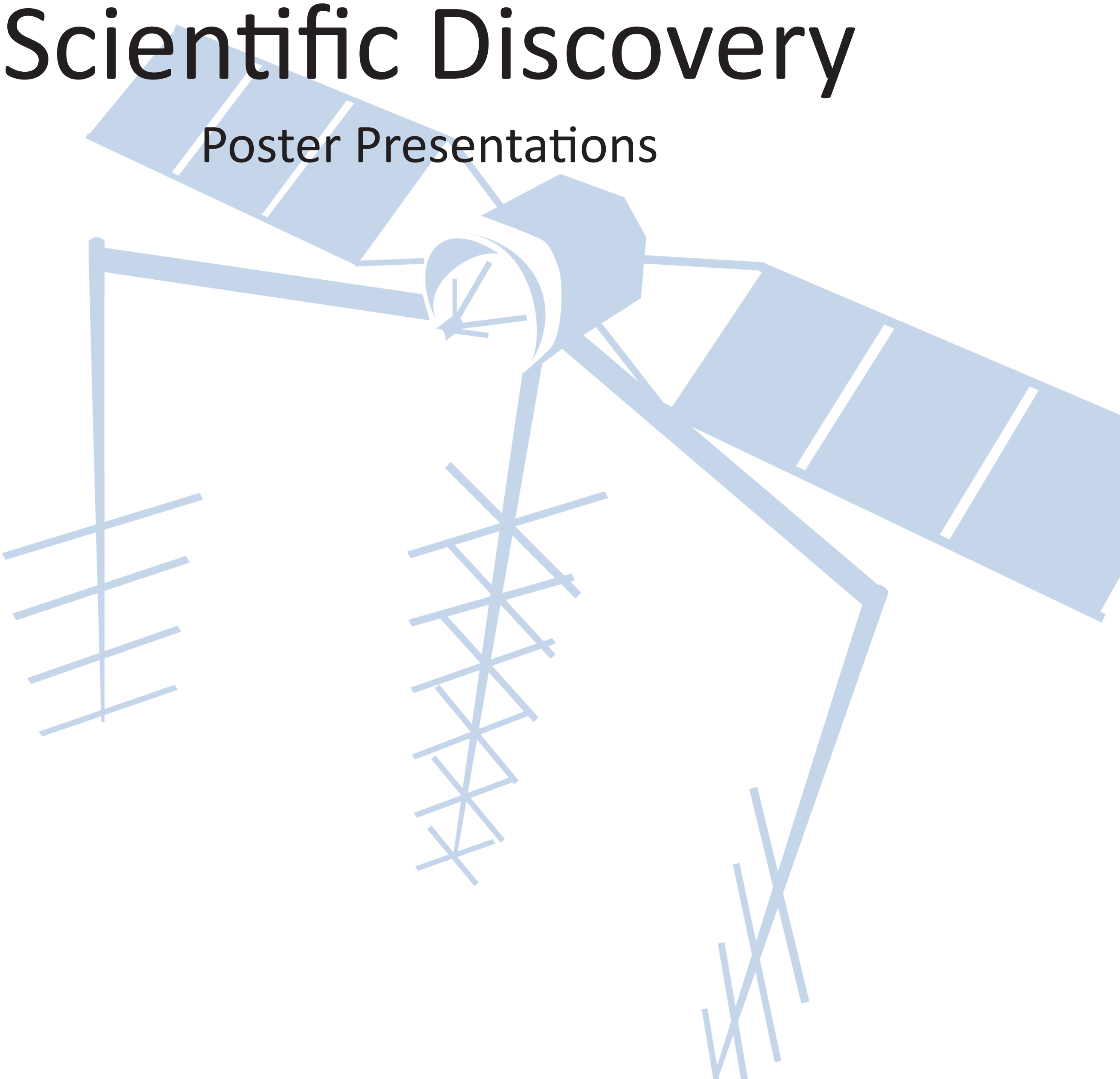
Luís Bettencourt (Principal Investigator), S. Brumby, G. Kenyon, J. George, C. Rasmussen, A. Galbraith, M. Anghel, and M. Ham

The Petascale Synthetic Visual Cognition LDRD-DR project is exploring how a human brain sees. To answer this question, we are using one of the world's most powerful computers, LANL's Roadrunner petaflop supercomputer, to build the world's first full-scale, real-time model of the part of human brain called visual cortex. Additionally, small mammals are capable of excellent visual acuity and object recognition with orders of magnitude smaller brains. New graphics-card based computing technology could enable widespread use of brain models for many computer vision tasks. We present initial results with our massively parallel brain models, and demonstrate finding vehicles in aerial video.

*We have preliminary results using a learned model of primary visual cortex on public-release UAV-like imagery of vehicle detection and tracking scenarios provided by the DARPA/DSO Neovision2 program.*

# Scientific Discovery

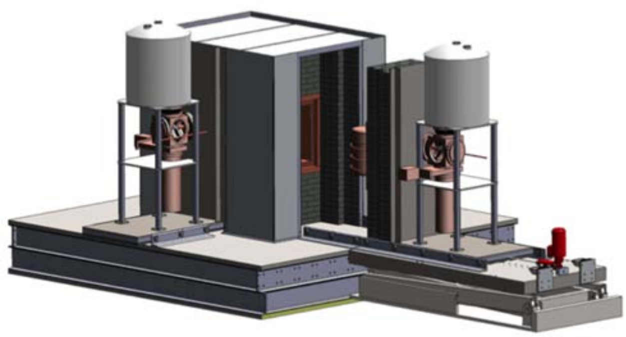
## Poster Presentations



## The Majorana Neutrinoless Double Beta Decay Experiment (Poster 38)

Melissa Boswell, M. Akashi-Ronquest, S. Elliott (Principal Investigator), V. Gehman, A. Hime, M. Kidd, K. Rielage, L. Rodriguez, H. Salazar, and D. Steele

In 1986, three scientists studying Selenium at the University of California Irvine observed an extremely rare form of nuclear disintegration, known as double beta decay. In this process the nucleus decays emitting two electrons and two antineutrinos. Those early methods are now being used to search for an even more rare decay mode known as neutrinoless double-beta decay, where no neutrinos are emitted and which can only occur if the neutrino is its own antiparticle. These measurements will provide valuable information on the relationship between the neutrino and its antiparticle, as well the information required for understanding the neutrino mass. The Majorana experiment proposes to assemble an array of High-purity Germanium (HPGe) detectors to search for neutrinoless double-beta decay in 76Ge. By using ultrapure materials, and housing the experiment 4,850 feet underground at the Sanford mine in South Dakota, the collaboration hopes to be sensitive to the few tens of neutrinoless double beta decay events that occur each year. In addition to providing a ground-breaking scientifc impact, neutrinoless double beta experiments are advancing technology frequently used in diagnostic and therapeutic medicine, as well as threat reduction. All of these fields rely on HPGe detectors to observe weak signals from radioactive materials. Information from low-background experiments such as Majorana will certainly provide the technology necessary for these other industries to reach unprecedented levels of sensitivity.



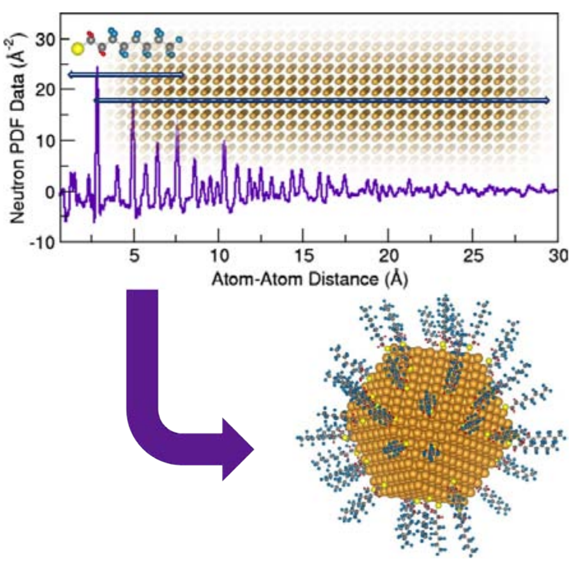
*Achieving the sensitivity required to search for neutrinoless double beta decay requires signifcant amounts of shielding, and the use of very radiopure materials. Shown here is a schematic of the Majorana Demonstrator.*

*The Demonstrator design currently consists of HPGe detectors encased in several inches of electroformed Cu, further surrounded by more layers of lead shielding. In order to reduce the effects of cosmic-rays, the entire system will be placed deep underground in a gold mine in South Dakota.*

## Building the Complete Nanoparticle Picture with Neutrons and High Energy X-rays (Poster 39)

Katharine Page (Postdoctoral Researcher), E. Tencate, and T. Proffen (Principal Investigator)

The diameter of a nanoparticle is smaller than 1/4,000th of a human hair. Scientists and engineers make them in a diverse set of shapes and architectures and they can have unique atomic structures or defects we do not find elsewhere in nature. These features provide novel physical properties, making them of tremendous interest for new technological innovations. However, very small size presents a real challenge when it comes to observing such details, requiring a new set of characterization tools. We describe advancements in neutron and high energy x-ray total scattering for the study of complete nanoparticle structures, with surprising results.




*The pair distribution function (PDF) from neutron total scattering data collected at LANL's Lujan Neutron Scattering Center contains information about every pair of atoms in a sample, allowing us to determine, for example, the complete atomic structure of ligand-capped gold nanoparticles.*

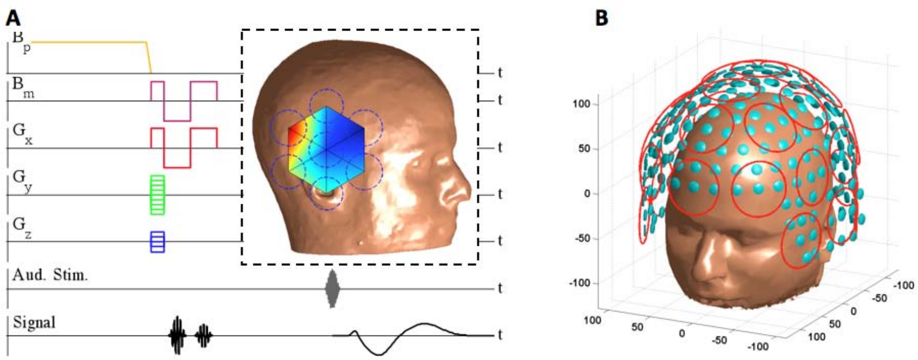
## Probing Brain Dynamics by Ultra-Low Field Magnetic Resonance (Poster 40)

Michelle Espy (Principal Investigator), J. George, A. Guthormsen, P. Magnelind, A. Matlashov, P. Volegov, and Los Alamos SQUID Team

In our efforts to experimentally measure the temporal and spatial dynamics of the human brain we have successfully completed interleaved ultra-low field (ULF) magnetic resonance imaging (MRI) and magnetoencephalography (MEG) measurements separated by about three seconds in time (see Figure A). The ULF-MRI provides structural information while the MEG provides a functional image. The time delay between the two measurement techniques is due to field-switching transients in the walls of the shielded room, in which the 7-channel system is operated.

Since the effect, which is used in functional MRI at high fields, is negligible at ultra-low fields, we are implementing an arterial spin-labeling technique. Coils for the necessary spin inversion are being designed. In order to improve the signal-to-noise ratio we have designed a set of pre-polarization coils which are going to generate a field of 0.2 T compared to our present 0.03 T field.

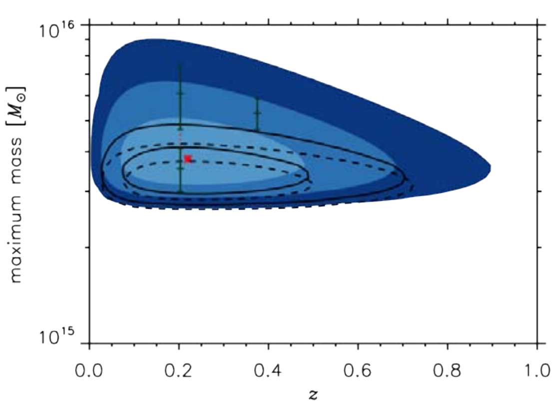
Moreover, we are currently trying to combine the high spatial resolution of functional MRI and anatomical MRI with the high temporal resolution of MEG. The high-resolution map obtained through anatomical MRI combined with the retinotopic map obtained via fMRI will be used to localize the MEG data. To increase the coverage of the whole cortex we will customize a commercial 122 channel MEG dewar to incorporate a number of MRI channels (see Figure B).




*A) Pulse sequence used for the interleaved ULF-MRI and MEG measurements with the resulting MEG map. B) Teal markers indicate the available MEG sensors in the 122 channel system and the red circles show the MRI channels that will be added to the existing system.*

## The Most Massive Objects in the Universe (Poster 41)

Daniel Holz (Principal Investigator), A. Heger, J. Jungman, S. Perimutter, and M. Warren

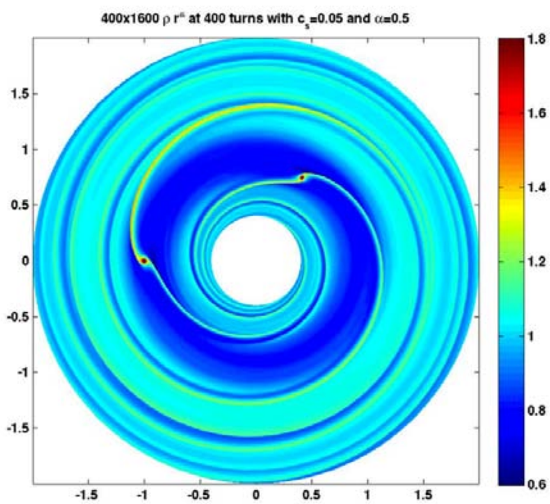



We calculate what should be the most massive object in the Universe: a supercluster of galaxies at roughly 5 billion lightyears away from us. By confirming this prediction, we can test the standard model of cosmology. If observations don't agree with predictions, this will be an indication that new physics is occurring in the very early Universe, or that gravity is "broken." We analyze recent data, and show that while some data agrees perfectly with predictions, there is also data that is in some tension.

*Contour plot of the most massive objects in the Universe, predicted to lie in the blue region. This tells us the mass of this object, as well as the redshift (which is a measure of distance in cosmology). The red star represents the most likely mass and distance to the most massive cluster. The solid line contours are for the second most massive halo, while the dashed line contours are for the third most massive halo.*

## Wonders and Challenges of Extrasolar Planets  (Poster 42)

Hui Li (Principal Investigator) and Shengtai Li



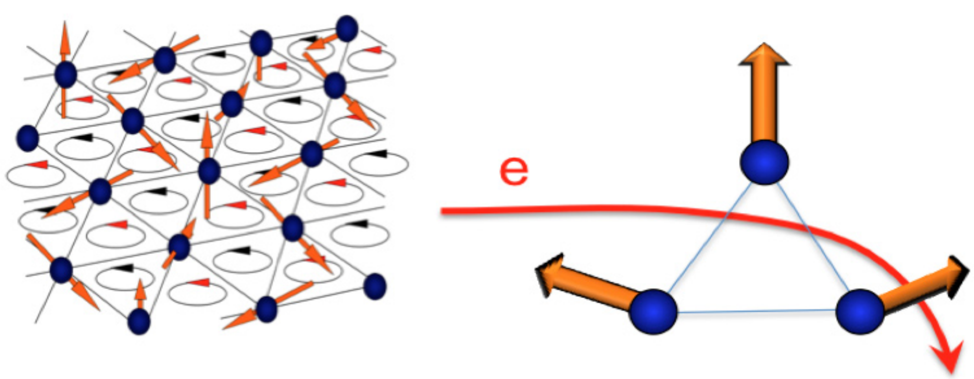

The exciting discoveries of more than 450 extra-solar planets (planets around other stars like our Sun) have generated enormous interests in public and scientific communities. Meanwhile, mysteries surrounding how these enigmatic systems form and evolve have captured the attention of astronomers and astrophysicists. To address some of the fundamental challenges presented by these discoveries, we have developed modern sophisticated computer codes to simulate the motion of these planets in their nascent disks around their parent star. Understanding the observations of these planets present both great challenges and opportunities to develop new, more advanced technologies for the Laboratory and the Nation.

*Two extra-solar planets are moving through a gaseous disk around a central star. The tidal forces from these planets drive the gas in the disk away from them (deep blue color region). With very little gas surrounding them, they no longer fall towards the central star. Instead, they stay at their orbits and survive the migration. The simulations were performed using our newly developed hydrodynamic computer code that runs on the supercomputers at Los Alamos.*

## Controlling Complex States Emerging from Frustration  (Poster 43)

Christian Batista, E. D. Bauer, I. Martin (Principal Investigator), J. D. Thompson, and V. Zapf

Functionalities provided by magnetism underpin our ability to compute and store huge bodies of information as well as to actuate and sense. Most of these technologies rely on ferromagnetism, i.e. the global parallel alignment of magnetic spins. In certain crystal structures, the alignment of spins can be frustrated. This leads to proximity of multiple stable complex magnetic states of matter, tunable by even a small perturbation in composition, pressure, or temperature, making frustrated systems fundamentally interesting and highly desirable for applications. Our objective is to pioneer a new direction for condensed matter science by discovering, understanding and controlling states that emerge from the coupling of itinerant charges to underlying frustrated spin textures.

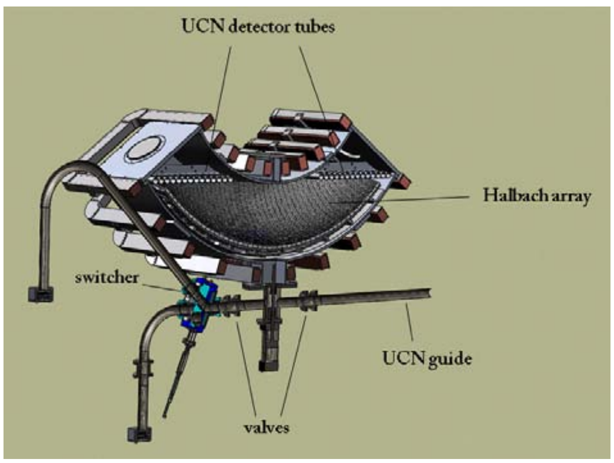



*Frustrated magnetic interactions lead to complex magnetic states (arrows indicate magnetic moments of individual atoms). When itinerant electron moves in such frustrated magnetic background, it experiences deflecting force equivalent to an astronomically high magnetic field.*

## Development of a Precise Measurement of the Neutron Lifetime (Poster 44)

Andy Saunders (Principal Investigator)

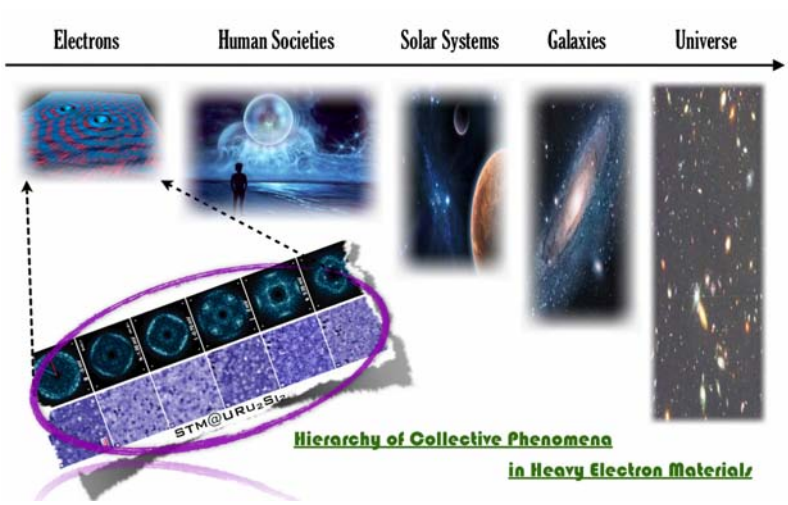
The neutron, although stable when confined in the nucleus of an atom, is unstable when free. The half-life is approximately 15 minutes, but is only known to a precision of about 1 second. The neutron lifetime has typically been measured by confining very low energy neutrons, called “ultra-cold” neutrons (UCN), in a material bottle, and then counting the survivors after different periods of time. Ultra-cold neutrons have the characteristic, unlike higher energy neutrons and other particles used in fundamental particle physics, that they can be totally reflected from common material surfaces, such as stainless steel, thus allowing them to be bottled like a gas for hundreds of seconds. Most recent previous measurements of the neutron lifetime have been plagued, though, by the complicated interactions between the neutrons and the walls of the storage bottles. We are constructing a new type of experiment, in which the neutron trap is constructed not of material walls but of magnetic walls (See Figure). The neutrons will interact with no materials at all after entering trap, thus eliminating systematic uncertainties associated with the material wall interactions. We expect to take first data with this experiment this year.




*The Los Alamos neutron lifetime experiment. The ultra-cold neutrons enter the magnetic trap, which is about the size and shape of a bathtub, from the bottom. Neutrons can be counted either in situ, using an external detector, or by detecting their decay products. In this cutaway view, the neutron detectors, the Halbach array of magnets forming the neutron trap, and the neutron fill tubes can all be seen.*

## Hierarchy of Collective Phenomena in Heavy Electron Materials (Poster 45)

Yi-feng Yang (Postdoctoral Researcher) and J. Thompson (Principal Investigator)




Just as trillions of cells make up human beings with intelligence, trillions of electrons exhibit a variety of collective phenomena. Heavy electron materials are such that electrons can become hundreds of times heavier than they usually are. They can also form superconducting pairs, flowing without costing energy. These are not only important for practical use, but also manifest a profound law of our universe: Emergence of new organizing principles of a large amount of interacting individuals that are different from those of individuals alone. We identify the hierarchy of scales governing the collective phenomena in heavy electron materials.

*Hierarchy of structure in our universe. Hierarchy of scales is also found in heavy electron materials, separating individual and collective behavior of electrons.*

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